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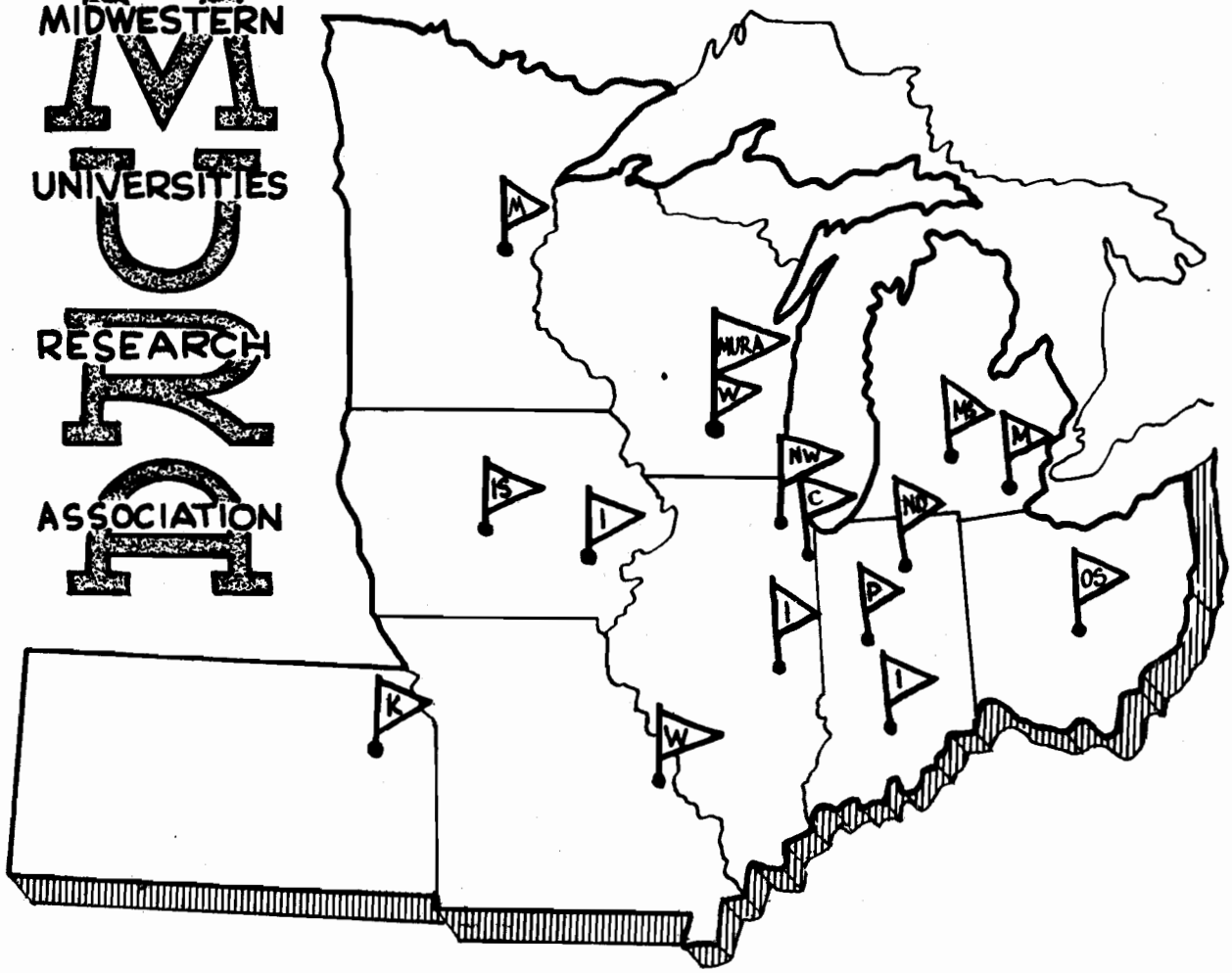

CONVERGENCE RATES OF ITERATIVE TREATMENTS OF LAPLACE'S EQUATION

REPORT **NUMBER** 327

MURA-327
Internal

MIDWESTERN UNIVERSITIES RESEARCH ASSOCIATION †

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CONVERGENCE RATES OF ITERATIVE TREATMENTS OF LAPLACE'S EQUATION

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June 28, 1957

ABSTRACT: The rates of convergence of the Richardson and Liebmann methods of solution of Laplace's equation in two and three dimensions are calculated.

† Supported by Contract AEC #AT (11-1) - 384

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INTRODUCTION

The possible need of a three-dimentional Laplace program in future work of MURA necessitates the examination of the rapidity of convergence of such a program and an estimation of the machine time required for a Laplace problem.

Frankel* has calculated convergence rates of the Richardson and Liebmann algorithms for two-dimentional Laplace problems for which the potential is specified on a rectangle. This is slightly different from the type of boundary value problem encountered in MURA work. In our problems the potential might be specified along the top and bottem edges of a rectangular region but not along the sides of the region. We would, instead, require the potential to be periodic in one direction with period equal to the bottom edge of the rectangle. Such boundary conditions will be referred to as "periodic boundary conditions" to be distinguished from the "fixed boundary conditions" of the type discussed by Frankel.

This report extends Frankel's work to three dimensions and includes the consideration of the potential periodic in one direction. These extensions are really quite simple but it seems worthwhile embodying them in a MURA report if only to fill in some of the gaps in Frankel's account of his work. In order to provide motivation for steps taken in the consideration of two- and three-dimensional problems, the one-dimensional problem is thoroughly discussed for both the Richardson and the Liebmann algorithms.

* S.P.Frankel, Mathematical Tables and Other Aids to Computation, 4, 65(1950).

1. Richardson Algorithm: One-dimensional Problem.

Consider the mesh shown in Figure 1.

Fig. 1

Let $\varphi_j^{(n)}$, $j=1,\cdots,N-1$, denote the calculated potential at point j after n iterations, the potential at the end points, $j=0$ and $j=N$, being fixed. The initial loading of the mesh is given by $\varphi_j^{(0)}$, $j=1,\cdots,N$. The Richardson algorithm is as follows:

$$\varphi_j^{(n+1)} = \frac{1}{2}\left(\varphi_{j-1}^{(n)} + \varphi_{j+1}^{(n)}\right) \quad , \quad j=1,\cdots,N-1 . \tag{1}$$

That is in each iteration the value of the potential at each point of the mesh is taken as the average of the potential values at the neighboring points for the previous iteration. This process converges to the solution of the one-dimensional Laplace equation, $\frac{d^2\varphi}{dx^2}=0$, satisfying the boundary conditions. Our question is how rapidly the process converges to this solution.

Rather than work with the potential itself, it is more convenient to work with the error of the potential, that is the deviation of the potential from its limiting value. Suppose that ϕ_j is the limiting value at point j of the potential yielded by the algorithm. Let $\epsilon_j^{(n)}$ be the error in the potential at point j after the nth iteration,

$$\epsilon_j^{(n)} = \varphi_j^{(n)} - \phi_j .$$

Since the iteration equations are linear, it is clear that these same equations hold for the $\epsilon_j^{(n)}$ with the boundary condition that $\epsilon_j^{(n)}$ is zero at the end points, $j=0$ and $j=N$.

Thus

$$\epsilon_j^{(n+1)} = \frac{1}{2}\left(\epsilon_{j-1}^{(n)} + \epsilon_{j+1}^{(n)}\right) \quad , \quad j=1,\cdots N-1 ,$$
$$\epsilon_0^{(n)} = \epsilon_N^{(n)} = 0 \quad , \quad \text{all } n . \tag{2}$$

Equation (2) can conveniently be written in matrix form,

$$\begin{pmatrix} \epsilon_1^{(m+1)} \\ \epsilon_2^{(m+1)} \\ \vdots \\ \epsilon_{N-1}^{(m+1)} \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ & & \ddots & \ddots & \\ & & & \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} \epsilon_1^{(m)} \\ \epsilon_2^{(m)} \\ \vdots \\ \epsilon_{N-1}^{(m)} \end{pmatrix} \tag{3}$$

or

$$E^{(m+1)} = L\, E^{(m)} \tag{4}$$

where the E's and the matrix L are shown explicitly in Eq.(3). If $E^{(0)}$ is the vector whose components are the errors in the potential at the initial loading of the mesh, then

$$E^{(m)} = L^{(m)} E^{(0)} \tag{5}$$

Let us suppose that L has a complete set of eigenvectors* $X_1, X_2, \ldots X_{N-1}$, with corresponding eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_{N-1}$. If we expand $E^{(0)}$ in this set, so that

$$E^{(0)} = \sum_{l=1}^{N-1} \alpha_l X_l \quad , \tag{6}$$

then Eq.(5) becomes

$$E^{(m)} = \sum_{l=1}^{N-1} \alpha_l \lambda_l^m X_l \quad . \tag{7}$$

If λ_m is the eigenvalue of greatest magnitude and is simple, then for large m

$$E^{(m)} \simeq \lambda_m^m \alpha_1 X_1 \quad . \tag{8}$$

---

* That L has a complete set of eigenvectors in this simple case is a necessary consequence of the symmetry of the matrix. In the discussion of the Liebmann algorithm we shall encounter matrices that do not have complete sets of eigenvectors.

Thus after a large number of iterations the rate of approach to the solution of the differential equation is determined by the largest (in magnitude) eigenvalue of L. If this eigenvalue is degenerate, or if L has another eigenvalue of the same magnitude but opposite sign, $E^{(m)}$ will still be proportional to $|\lambda_m|^m$.

The lapse rate, μ, in decades per iteration is given by

$$\mu = -\log|\lambda_m| \tag{9}$$

The problem has become one of determining the largest eigenvalue of L. The secular equation for is

$$D_{N-1}(\lambda) = \begin{vmatrix} -\lambda & \frac{1}{2} & & & \\ \frac{1}{2} & -\lambda & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \frac{1}{2} \\ & & & \frac{1}{2} & -\lambda \end{vmatrix} = 0 \quad , \tag{10}$$

the determinant D_{N-1} having $N-1$ rows and columns. The determinant can be expanded as follows. If we expand along the first row we obtain the recurrence relation

$$D_{N-1} = -\lambda D_{N-2} - \frac{1}{4} D_{N-3} \tag{11}$$

where D_{N-2} and D_{N-3} are determinants having the same form as , but with $N-2$ rows and $N-3$ rows, respectively. Eq.(11) is a linear differance equation with constant coefficients and can be solved by the same means used for linear differential equations with constant coefficients. Put

$$D_N = \nu^N \tag{12}$$

substitution of Eq.(12) into Eq.(11) yields

$$\nu^2 = -\lambda\nu - \frac{1}{4} \tag{13}$$

Thus

$$\nu = \frac{1}{2}\left\{-\lambda \pm \left[\lambda^2 - 1\right]^{\frac{1}{2}}\right\} \tag{14}$$

Eq.(14) and the equations to follow assume a particuarly simple form if we put

$$\lambda = \cos\vartheta \tag{15}$$

for then

$$\begin{aligned} \nu &= \frac{1}{2}\left\{-\cos\theta \pm i\sin\theta\right\} \\ &= -\frac{1}{2}e^{\pm i\theta} \end{aligned} \tag{16}$$

The general solution of Eq.(11) is therefore

$$D_N = A\left(-\tfrac{1}{2}\right)^N e^{iN\theta} + B\left(-\tfrac{1}{2}\right)^N e^{-iN\theta} \tag{17}$$

D_N must, however, satisfy the "initial conditions"

$$\begin{aligned} D_1 &= |-\lambda| = -\cos\vartheta \\ D_2 &= \begin{vmatrix} -\lambda & \frac{1}{2} \\ \frac{1}{2} & -\lambda \end{vmatrix} = \lambda^2 - \frac{1}{4} = \cos^2\theta - \frac{1}{4} \end{aligned} \tag{18}$$

and these conditions will determine A and B.

Thus, with $N = 1, 2$ in Eq.(17) we obtain

$$\begin{aligned} -\frac{1}{2}Ae^{i\theta} - \frac{1}{2}Be^{-i\theta} &= -\cos\theta \\ \frac{1}{4}Ae^{2i\theta} + \frac{1}{4}Be^{-2i\theta} &= \cos^2\theta - \frac{1}{4} \end{aligned} \tag{19}$$

The solution of these equations is

$$A = \frac{e^{i\theta}}{2i\sin\theta}, \quad B = -\frac{e^{-i\theta}}{2i\sin\theta}, \tag{20}$$

and so Eq.(17) becomes

$$D_N = \left(-\tfrac{1}{2}\right)^N \frac{\sin (N+1)\vartheta}{\sin \vartheta} \quad . \tag{21}$$

The roots of the secular equation, Eq.(10), are now easily determined. We have

$$D_{N-1} = \left(-\tfrac{1}{2}\right)^{N-1} \frac{\sin N\vartheta}{\sin \vartheta} \tag{22}$$

and so the roots are given by

$$\lambda_r = \cos \vartheta_r \quad , \quad \vartheta_r = \frac{2\pi}{N} r \quad , \quad r = 1, \ldots , N-1 \quad . \tag{23}$$

The root of largest magnitude is

$$\begin{aligned} \lambda_1 = |\lambda_{N-1}| &= \cos \frac{\pi}{N} \\ &\simeq 1 - \frac{1}{2}\left(\frac{\pi}{N}\right)^2 \end{aligned} \tag{24}$$

,

and the lapse rate, in decades per iteration, is therefore

$$\begin{aligned} \mu &= -\log\left(\cos \frac{\pi}{N}\right) \\ &\simeq \frac{1}{\ln 10} \cdot \frac{1}{2}\left(\frac{\pi}{N}\right)^2 \end{aligned} \tag{25}$$

.

It is instructive to obtain the eigenvectors of L . The equations satisfied by the components of the eigenvector belonging to the eigenvalue λ are

$$\begin{aligned} \tfrac{1}{2} x_2 &= \lambda x_1 \quad , \\ \tfrac{1}{2} x_{n-1} + \tfrac{1}{2} x_{n+1} &= \lambda x_n \quad , \qquad n = 2, \ldots N-2 , \\ \tfrac{1}{2} x_{N-2} &= \lambda x_{N-1} \quad . \end{aligned} \tag{26}$$

By introducing an x_0 and an x_N we can write these equations as follows:

$$\frac{1}{2}x_{n-1} + \frac{1}{2}x_{n+1} = \lambda x_n, \qquad n = 1, \cdots, N-1 \quad , \tag{27}$$

$$x_0 = x_N = 0 \quad .$$

(This technique of introducing additional variables satisfying boundary conditions in order to put the equations into a more symmetrical form will be used repeatedly in the later sections.) Eqs.(27) constitute a linear difference equation with constant coefficients which is easily solved. It isamusing, however, to make the substitution

$$x_n = (-2)^n y_n \tag{28}$$

for then Eq.(27) assumes the form

$$\lambda y_n = -y_{n+1} - \frac{1}{4} y_{n-1} \tag{29}$$

which is identical with Eq.(11), the difference equation satisfied by the determinants D_n . We have already obtained the general solution of this difference equation which, with a convenient normalization, yields

$$y_n = \left(-\frac{1}{2}\right)^n \sin n\theta \quad , \quad \lambda = \cos\theta , \tag{30}$$

satisfying the boundary conditions. Thus

$$x_n = \sin n\theta_r \qquad \text{if} \quad \lambda = \cos\theta_r \tag{31}$$

These $(N-1)$ eigenvectors form a complete set.

2. Richardson Algorithm: Two-dimensional Problem, Fixed Boundary Conditions

This is the case treated by Frankel, but we can briefly retrace his steps with the insight and motovation provided by our discussion of the one-dimensional problem.

Consider a rectanglar mesh of points distinguished by a pair of coordinates, i and j, where i takes on integral values from 0 to N_1 and j takes on integral values from 0 to N_2. The algorithm then yields for the errors in the potential, corresponding to Eq.(2) in the one-dimensional case,

$$\epsilon_{ij}^{(m+1)} = \frac{1}{4}\left(\epsilon_{i-1,j}^{(m)} + \epsilon_{i,j-1}^{(m)} + \epsilon_{i+1,j}^{(m)} + \epsilon_{i,j+1}^{(m)}\right),$$
$$\epsilon_{i0}^{(m)} = \epsilon_{iN_2}^{(m)} = \epsilon_{0j}^{(m)} = \epsilon_{N_1 j}^{(m)} = 0 \quad , \text{all } m . \tag{32}$$

If we think of the $\epsilon^{(m)}$'s for the interior point of the mesh as forming the components of a vector, $E^{(m)}$, in an $(N_1-1)\times(N_2-1)$-dimensional space, then Eq.(32) can be written as

$$E^{(m+1)} = L\, E^{(m)} \tag{33}$$

where L is a matrix whose ~~components~~ elements are all either 0 or $\frac{1}{4}$. One can, if one wishes, write down the matrix L if one chooses some convenient way of ordering the rows and columns. This, however, is not very illuminating, as is usually the case for problems referring to more than one dimension.

The general discussion contained in the paragraph following Eq.(5) applies to the two- and three-dimensional cases as well as to the one-dimensional case. Thus what is desired is the eigenvalue of L of largest magnitude, λ_m, the lapse rate being given by Eq.(9).

The easiest way to solve this problem is to use the experience gained in the treatment of the one-dimensional case in order to make an informed "guess" of the eigenvectors of L. The equations to be satisfied are

$$\lambda x_{ij} = \frac{1}{4}\left(x_{i-1,j} + x_{i,j-1} + x_{i+1,j} + x_{i,j+1}\right), \qquad i = 1, \cdots N_1 - 1, \qquad j = 1, \cdots N_2 - 1, \tag{34}$$

$$x_{0j} = x_{N_1 j} = x_{i0} = x_{iN_2} = 0 \quad .$$

These equations correspond to Eqs.(27) in the one-dimensional case. Taking our cue from Eq.(31) we try as the solution of these equations

$$x_{ij} = \sin i\theta_1 \sin j\theta_2 \tag{35}$$

where, in order that the boundary conditions at $i = N_1$ and $j = N_2$ be satisfied,

$$\theta_1 = \frac{\pi}{N_1} r \quad , \quad \theta_2 = \frac{\pi}{N_2} s \quad . \tag{36}$$

These vectors form a complete set in the space of $(N_1 - 1)\cdot(N_2 - 1)$ dimensions. The substitution of Eq.(35) into Eq.(34) yields, after some manipulation,

$$\lambda = \frac{1}{2}\left(\cos\theta_1 + \cos\theta_2\right) \quad . \tag{37}$$

The eigenvalue of largest magnitude is

$$\lambda_{max} = \frac{1}{2}\left(\cos\frac{\pi}{N_1} + \cos\frac{\pi}{N_2}\right) \approx 1 - \frac{1}{4}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2\right] \tag{38}$$

and the lapse rate in decades per iteration is

$$\mu = -\log\left\{\frac{1}{2}\left(\cos\frac{\pi}{N_1} + \cos\frac{\pi}{N_2}\right)\right\} = \frac{1}{\ln 10}\cdot\frac{1}{4}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2\right] . \tag{39}$$

3. Richardson Algorithm: Three-dimensional Problem; Fixed Boundary Conditions

The three-dimensional problem leads to no special difficulties. The analysis proceeds in a manner exactly parallel to the two-dimensional case and leads to the result

$$\begin{aligned}\lambda_{max} &= \frac{1}{3}\left(\cos\frac{\pi}{N_1} + \cos\frac{\pi}{N_2} + \cos\frac{\pi}{N_3}\right) \\ &\simeq 1 - \frac{1}{6}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right]\end{aligned} \tag{40}$$

where N_1+1, N_2+1, N_3+1 are the dimensions of mesh including the rectangular parallelepipedal boundary. The corresponding lapse rate is

$$\begin{aligned}\mu &= -\log\left\{\frac{1}{3}\left(\cos\frac{\pi}{N_1} + \cos\frac{\pi}{N_2} + \cos\frac{\pi}{N_3}\right)\right\} \\ &\simeq \frac{1}{\ln 10}\cdot\frac{1}{6}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right].\end{aligned} \tag{41}$$

4. Richardson Algorithm: Two-dimensional Problem; Periodic Boundary Conditions

We consider a rectangular mesh of points distinguished by a pair of coordinates i and j where i takes on integral values from 0 to N_1 and j takes on integral values from 0 to N_2. This mesh is to be thought of as being wrapped around a cylinder whose axis is in the direction of increasing j. The coordinate i can then assume all integral values but we must understand that points with the same value of j whose i-coordinates differ by a multiple of N_1 are identical. In short, we seek solutions of Laplace's equation for which the potential is periodic in one direction with period N_1. The potential is given at the surfaces $j=0$ and $j=N_2$. The Richardson Algorithm then yields

$$\varphi_{ij}^{(m+1)} = \frac{1}{4}\left(\varphi_{i-1,j}^{(m)} + \varphi_{i,j-1}^{(m)} + \varphi_{i+1,j}^{(m)} + \varphi_{i,j+1}^{(m)}\right) \tag{42}$$

subject to the boundary conditions

$$\varphi_{i0}^{(n)} = \phi(x=i, y=0) \quad , \quad \varphi_{iN_2}^{(n)} = \phi(x=i, y=N_2) \, ,$$
$$\varphi_{ij}^{(n)} = \varphi_{i+N_1,\, j}^{(n)} \quad , \qquad \text{all } i \text{ and } n \, , \tag{43}$$

where $\phi(i,0)$ and $\phi(i,N_2)$ are the prescribed boundary values of the potential. The equations and boundary conditions satisfied by the deviations of the calculated potential at the mesh points from the limiting values yielded by the algorithm are

$$\epsilon_{ij}^{(n+1)} = \frac{1}{4}\left(\epsilon_{i-1,j}^{(n)} + \epsilon_{i,j-1}^{(n)} + \epsilon_{i+1,j}^{(n)} + \epsilon_{i,j+1}^{(n)}\right) \quad \begin{matrix} i=1,\cdots,N_1, \\ j=1,\cdots N_2-1, \end{matrix} \tag{44}$$
$$\epsilon_{i0}^{(n)} = \epsilon_{iN_2}^{(n)} = 0 \, , \quad \epsilon_{ij}^{(n)} = \epsilon_{i+N_1,\, j}^{(n)} \quad , \qquad \text{all } i, \; j, \; n \, .$$

These equations can be written in the form of Eq. (5) in which L is a matrix with $N_1 \cdot (N_2-1)$ rows and columns. Once again we want to find the eigenvalue of L of largest magnitude, and again the easiest approach is to guess at a complete set of solutions of the equations

$$\lambda x_{ij} = \frac{1}{4}\left(x_{i-1,j} + x_{i,j-1} + x_{i+1,j} + x_{i,j+1}\right) , \quad i=1,\cdots N_1 , \; j=1,\cdots N_2-1 , \tag{45}$$
$$x_{i0} = x_{iN_2} = 0 \quad , \quad x_{ij} = x_{i+N_1,\, j} \, .$$

Note that except for the equations referring to points on the boundary of the mesh, $i=1$ and $i=N_2$, Eqs. (45) are identical with Eqs. (34). It must then follow that any solutions of Eq. (34) that satisfy the boundary conditions contained in Eqs. (45) will be solutions of Eqs. (45). Eqs. (35) and (36) provide such solutions for those values of θ_1 for which r is even. These solutions are

$$x_{ij} = \sin i\theta_1 \sin j\theta_2 \, ,$$
$$\theta_1 = \frac{\pi}{N_1} r \quad , \qquad r = 2, 4, \cdots , \begin{cases} N_1-2 & \text{if } N_1 \text{ is even} \\ N_1-1 & \text{if } N_1 \text{ is odd} \end{cases} \tag{46}$$
$$\theta_2 = \frac{\pi}{N_2} s \quad , \qquad s = 1, 2, \cdots , N_2-1 \, .$$

There are $\frac{(N_1-2)}{2}\cdot(N_2-1)$ such solutions if N_1 is even, and $\frac{(N_1-1)}{2}\cdot(N_2-1)$ of them if N_1 is odd. The corresponding eigenvalues are

$$\lambda = \frac{1}{2}\left(\cos\theta_1 + \cos\theta_2\right) .$$

One can surmise what the remaining solutions must be by noting that the solutions given by Eqs.(46) are all antisymmetrical about the center of the mesh. They are sinusoids whose periods in the i-direction are integral sub-multiples of the basic period N_1. We are therefore led to try

$$x_{ij} = \cos i\theta_1 \sin j\theta_2 \tag{47}$$

as solutions, where the boundary conditions require that

$$\theta_1 = \frac{\pi}{N_1} r \quad , \quad r = 0, 2, 4, \ldots \begin{cases} N_1 & \text{if } N_1 \text{ is even} \\ N_1 - 1 & \text{if } N_1 \text{ is odd} \end{cases} , \tag{48}$$

$$\theta_2 = \frac{\pi}{N_2} s \quad , \quad s = 1, 2, \ldots N_2 - 1 .$$

Substitution of Eq.(47) into Eqs.(45) shows that these are indeed solutions provided that

$$\lambda = \frac{1}{2}\left(\cos\theta_1 + \cos\theta_2\right) , \tag{49}$$

as before. There are $\frac{(N_1+2)}{2}\cdot(N_2-1)$ such solutions if N_1 is even, and $\frac{(N_1+1)}{2}\cdot(N_2-1)$ such solutions if N_1 is odd. These solutions and the antisymmetrical ones given by Eq.(46) are linearly independent of each other(they are, infact, orthogonal) and their total number is just $N_1(N_2-1)$ so that they form a complete set. It may be noted that aside from accidential degeneracies(occuring, for example, when $N_1 = N_2$) the eigenvalues are two-fold degenerate except for those having $\theta_1 = 0$ and $\theta_2 = \pi$ (the latter occurring only when N_1 is even).

That eigenvalue is a maximum for which $\theta_1 = 0$ and $\theta_2 = \frac{\pi}{N_2}$. Thus

$$\begin{aligned} \lambda_{max} &= \frac{1}{2}\left(1 + \cos\frac{\pi}{N_2}\right) \\ &\simeq 1 - \frac{1}{4}\left(\frac{\pi}{N_2}\right)^2 \end{aligned} \tag{50}$$

and the lapse rate in decades per sector is

$$\mu = -\log\left\{\tfrac{1}{2}\left(1+\cos\tfrac{\pi}{N_2}\right)\right\} \cong \frac{1}{\ln 10}\,\frac{1}{4}\left(\frac{\pi}{N_2}\right)^2, \tag{51}$$

independent of N_1. If N_1 is even then $\theta_1 = \pi$, $\theta_2 = \frac{\pi}{N_2}(N_2-1)$ yields a negative eigenvalue of the same magnitude as λ_{max}. If N_1 is much greater than N_2 there is very little difference between this result and the lapse rate for the case of fixed boundary conditions. If, however, N_1 is about as large as N_2 then the convergence of the algorithm for the periodic problem will be about half as swift as the convergence for the problem with fixed boundary conditions. This dependence of the lapse rate on only one dimension of the mesh resembles a phenomenon observed in calculations performed at Los Alamos. There a Laplace problem was solved for a rectangular region for which the potential was specified on one pair of sides and the normal derivative of the potential was specified on the other pair of sides. It was found that when the potential was specified on the shorter sides the lapse rate was much lower than it was for a problem with the potential specified on the long sides. It is shown in Appendix I that this problem is equivalent to one with periodic boundary conditions and the phenomenon seems to be accounted for by our results.

5. Richardson Algorithm: Three-dimensional Problem; Periodic Boundary Conditions

It is fairly obvious what the result of this calculation must be. We consider a mesh of points defined by the coordinates i, j, k, where i assumes integral values from 0 to N_1, j assumes integral values from 0 to N_2 and k assumes integral values from 0 to N_3. If the sought for solution of Laplace's equation is to be periodic in one direction, say the i-direction, then the lapse rate is given by

$$\mu = \frac{1}{\ln 10} \cdot \frac{1}{6} \left[\left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2 \right] . \tag{52}$$

If the sought for solution is to be periodic in two directions, the i- and j-directions, let us say, then the lapse rate is given by

$$\mu = \frac{1}{\ln 10} \cdot \frac{1}{6} \left(\frac{\pi}{N_3}\right)^2 . \tag{53}$$

6. Liebmann Algorithm: One-dimensional Problem.

We consider a mesh of points, $x = j$ where $j = 0, 1, \ldots, N$, initially loaded with potential values $\varphi_j^{(0)}$ with φ_0 and φ_N fixed by the boundary conditions of the problem. The Liebmann algorithm differs from the Richardson algorithm in that in a given iteration it makes use of values already computed in the course of that iteration. The algorithm is given by

$$\begin{aligned} \varphi_j^{(n+1)} &= \tfrac{1}{2}\left(\varphi_{j-1}^{(n+1)} + \varphi_{j+1}^{(n)}\right), \quad j = 1, 2, \cdots, N-1, \\ \varphi_0^{(n)} &= \phi(x=0), \quad \varphi_N^{(n)} = \phi(x=N) \quad \text{for all } n, \end{aligned} \tag{54}$$

where $\phi(0)$ and $\phi(N)$ are the prescribed boundary values. For the deviations of the potential from the limiting values yielded by the algorithm one has

$$\begin{aligned} \epsilon_j^{(n+1)} &= \tfrac{1}{2}\left(\epsilon_{j-1}^{(n+1)} + \epsilon_{j+1}^{(n)}\right), \quad j = 1, \cdots, N-1, \\ \epsilon_0^{(n)} &= \epsilon_N^{(n)} = 0 \quad \text{for all } n. \end{aligned} \tag{55}$$

If each of these equations is solved in turn for $\epsilon_j^{(n+1)}$ and substituted into the succeeding equation one obtains

$$\begin{aligned} \epsilon_1^{(n+1)} &= \tfrac{1}{2}\epsilon_2^{(n)} \\ \epsilon_2^{(n+1)} &= \tfrac{1}{4}\epsilon_2^{(n)} + \tfrac{1}{2}\epsilon_3^{(n)} \\ &\vdots \\ \epsilon_{N-2}^{(n+1)} &= \left(\tfrac{1}{2}\right)^{N-2}\epsilon_2^{(n)} + \left(\tfrac{1}{2}\right)^{N-3}\epsilon_3^{(n)} + \cdots + \tfrac{1}{2}\epsilon_{N-1}^{(n)} \\ \epsilon_{N-1}^{(n+1)} &= \left(\tfrac{1}{2}\right)^{N-1}\epsilon_2^{(n)} + \left(\tfrac{1}{2}\right)^{N-2}\epsilon_3^{(n)} + \cdots + \tfrac{1}{4}\epsilon_{N-1}^{(n)} \end{aligned} \tag{56}$$

or

$$E^{(m+1)} = L\,E^{(m)} \tag{57}$$

where

$$L = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & 0 & \cdots & 0 & 0 \\ 0 & \frac{1}{8} & \frac{1}{4} & \frac{1}{2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & \left(\frac{1}{2}\right)^{N-2} & \left(\frac{1}{2}\right)^{N-3} & \left(\frac{1}{2}\right)^{N-4} & \cdots & \frac{1}{4} & \frac{1}{2} \\ 0 & \left(\frac{1}{2}\right)^{N-1} & \left(\frac{1}{2}\right)^{N-2} & \left(\frac{1}{2}\right)^{N-3} & \cdots & \frac{1}{8} & \frac{1}{4} \end{pmatrix} \tag{58}$$

If L has a complete set of eigenvectors then the argument following Eq.(5) holds and the lapse rate is calculated from the eigenvalue of largest magnitude. Here, unlike the case of the Richardson algorithm, L is not a symmetric matrix and the completeness of its eigenvectors is by no means assured. We will find, in fact, that the eigenvectors of L do not form a complete set, a circumstance necessitating a supplementation of the argument following Eq.(5).

We want to solve the problem

$$LX = \lambda X \tag{59}$$

where L is given by Eq.(58). There seems to be no convenient way to handle this problem directly because L has a fairly complicated form. Suppose we had a non-singular matrix S such that SL had a simple form. We could then find the eigenvalues of L by multiplying Eq.(59) by S, yielding

$$(SL - \lambda S)X = 0 \tag{60}$$

and solving the secular equation

$$
\begin{aligned}
0 &= |SL - \lambda S| \\
&= |S| \cdot |L - \lambda \mathbf{1}|
\end{aligned}
\tag{61}
$$

The solutions of this secular equation are precisely the eigenvalues of L. Futhermore the solutions, X, of Eq.(60) are the same as the solutions of Eq.(59), again as a consequence of the non-singularity of S. For S choose

$$
S = \begin{pmatrix} 2 & & & & \\ -1 & 2 & & 0 & \\ & -1 & 2 & & \\ & & \ddots & \ddots & \\ & 0 & & -1 & 2 \end{pmatrix}
\tag{62}
$$

which is obviously non-singular, having determinant 2^{N-1}.

Then

$$
SL = \begin{pmatrix} 0 & 1 & & & \\ & 0 & 1 & & 0 \\ & & 0 & \ddots & \\ & & & \ddots & 1 \\ & 0 & & & 0 \end{pmatrix}
\tag{63}
$$

and

$$SL - \lambda S = \begin{pmatrix} -2\lambda & 1 & & & 0 \\ \lambda & -2\lambda & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ 0 & & & \lambda & -2\lambda \end{pmatrix} , \tag{64}$$

We want the solution of

$$Q_{N-1}(\lambda) = |SL - \lambda S| = 0 , \tag{65}$$

and can obtain these solutions by the same sort of procedure that was used to solve Eq.(10). If the determinant Q_{N-1} is expanded along its first row one obtains

$$Q_{N-1} = -2\lambda Q_{N-2} - \lambda Q_{N-3} \tag{66}$$

where Q_{N-2} and Q_{N-3} are determinants of the same form as Q_{N-1} but having $N-2$ and $N-3$ rows respectively. Eq.(66) constitutes a second-order difference equation for the Q's subject to the initial conditions

$$Q_1 = |-2\lambda| = -2\lambda ,$$
$$Q_2 = \begin{vmatrix} -2\lambda & 1 \\ \lambda & -2\lambda \end{vmatrix} = 4\lambda^2 - \lambda . \tag{67}$$

Put

$$Q_N = \nu^N . \tag{68}$$

Then substitution of Eq.(68) into Eq.(66) yields

$$\nu^2 + 2\lambda\nu + \lambda = 0$$

which has the solutions

$$\nu = -\lambda \pm [\lambda^2 - \lambda]^{\frac{1}{2}} . \tag{69}$$

If we put

$$\lambda = \cos^2\vartheta \tag{70}$$

then these solutions become

$$\nu = -\cos\vartheta \; e^{\pm i\vartheta} \quad . \tag{71}$$

The general solution of Eq.(66) is therefore

$$Q_N = (-1)^N \cos^N\vartheta \left\{ A e^{iN\vartheta} + B e^{-iN\vartheta} \right\} \quad . \tag{72}$$

The coefficients, A and B, are determined by the initial conditions, Eqs.(67), and one obtains after some simple algebra

$$A = \frac{e^{i\vartheta}}{2i\sin\vartheta} \quad , \quad B = -\frac{e^{-i\vartheta}}{2i\sin\vartheta} \quad , \tag{73}$$

whence

$$Q_{N-1} = (-1)^{N-1} \cos^{N-1}\vartheta \; \frac{\sin N\vartheta}{\sin\vartheta} \quad . \tag{74}$$

The distinct solutions of Eq.(65) are given by

$$\left.\begin{aligned} \vartheta &= \frac{\pi}{N} r \\ \lambda &= \cos^2 \frac{\pi}{N} r \end{aligned}\right\} \quad , \qquad r = 1, 2, \cdots, \begin{cases} \frac{N}{2} - 1 & \text{if } N \text{ is even} \\ \frac{N-1}{2} & \text{if } N \text{ is odd} \end{cases}$$

$$\left.\begin{aligned} \vartheta &= \frac{\pi}{2} \\ \lambda &= 0 \end{aligned}\right\} \qquad \begin{aligned} &\text{an } \tfrac{N}{2}\text{-fold root if } N \text{ is even,} \\ &\text{an } \tfrac{N-1}{2}\text{-fold root if } N \text{ is odd.} \end{aligned} \tag{75}$$

It has already been pointed out that the eigenvectors of L are the solutions of Eq.(60). With $SL - \lambda S$ as given by Eq.(64), Eq.(60) can be written

$$\begin{aligned} \lambda x_{n-2} - 2\lambda x_{n-1} + x_n &= 0 \quad , \quad n = 2, \cdots, N, \\ x_0 = x_N &= 0 \quad . \end{aligned} \tag{76}$$

This equation bears a marked resemblance to Eq.(66). In fact, if we

substitute

$$x_n = (-1)^{n-1} Q_{n-1}(\lambda) \tag{77}$$

into Eq. (76) we obtain

$$\lambda Q_{n-3} + 2\lambda Q_{n-2} + Q_{n-1} = 0 \tag{78}$$

which is identical with Eq. (66) . We have already obtained a special solution of Eq. (66) , namely Eq. (74) . Futhermore this special solution when used in Eq. (77) yields a solution of Eq. (76) satisfying the boundary conditions appended to Eq. (76) since $Q_{-1}(\lambda) = 0$ and $Q_{N-1}(\lambda) = 0$ by virtue of the fact that λ satisfies Eq. (65) .

The solutions given by Eq. (77) form a set of linearly independent eigenvectors of L belonging to the non-zero eigenvalues of L . What of the highly multiple root $\lambda = 0$? Examination of Eq. (76) makes it clear that corresponding to $\lambda = 0$ there is only one eigenvector, namely,

$$x_1 \neq 0 \ , \quad x_n = 0 \quad \text{if } n \neq 1 \ .$$

Consequently L does not have a complete set of eigenvectors and the argument following Eq. (5) breaks down. L has, infact, just $\frac{N}{2}$ eigenvectors if N is even, and $\frac{N+1}{2}$ eigenvectors if N is odd. If the initial set of errors in the potential, $E^{(0)}$, were expandable in eigenvectors of L then the general argument would apply, but if $E^{(0)}$ has a non-vanishing projection into that part of the $(N-1)$ -dimensional vector space that is not spanned by eigenvectors of L, we do not know that Eq. (9) is correct. This situation is met by the following theorem which is proved in Appendix II. *

---

* It has been pointed out by Homer Meier that this theorem is a trivial consequence of the theorem that every matrix can be transformed into the Jordan canonical form. The self-contained proof presented in Appendix II is included in the report anyway in the event that the reader is as unfamiliar with this aspect of matrix theory as the authors were.

<u>Theorem</u>: T is an $n \times n$ matrix with linearly independent eigenvectors $X_1, \cdots X_r$ $(r<n)$ and corresponding eigenvalues $\lambda_1, \cdots, \lambda_r$ (not necessarily distinct and not necessarily non-zero). In addition to these eigenvalues the secular equation of T has a root $\lambda = 0$ of multiplicity $n-r$. If Z is a vector orthogonal to $X_1, \cdots, X_r$ then $T^{n-r} Z = 0$.

An example illustrating the above theorem is given by the matrix

$$T = \begin{pmatrix} 0 & 1 & & & 0 \\ & 0 & 1 & & \\ & & 0 & 1 & \\ & & & \ddots & \ddots \\ 0 & & & & 1 \\ & & & & 0 \end{pmatrix}_n$$

whose secular equation is $(-\lambda)^n = 0$. This matrix has only one eigenvector, $[X]_i = x_1 \delta_{1i}$, so that only for this vector is it true that $TX = 0$. But for an arbitrary vector Y it is readily seen that $T^n Y = 0$.

The significance of this theorem for our work is that although the initial set of errors, $E^{(0)}$, do not conform to the conditions necessary for the applicability of our general argument ($E^{(0)}$ expandable in eigenvectors of L), a finite number of iterations suffice to produce a set of errors that do conform to our requirements. The number of iterations necessary is one less than the multiplicity of the root $\lambda = 0$ (one less because there is one eigenvector belonging to this root). The multiplicity of this root is given in Eq.(75). Since under ordinary circumstances the number of iterations used in any given problem will be much larger than N, the incompleteness of the eigenvectors of L produces no delay in the convergence of the algorithm and the lapse rate is correctly given by Eq.(9).

According to Eq.(75)

$$\begin{aligned} \lambda_{max} &= \cos^2 \frac{\pi}{N} \\ &\simeq 1 - \left(\frac{\pi}{N}\right)^2 \end{aligned} \tag{79}$$

and so

$$\mu = -\log\left(\cos^2 \frac{\pi}{N}\right)$$
$$\simeq \frac{1}{\ln 10} \cdot \left(\frac{\pi}{N}\right)^2 \tag{80}$$

This is just twice the result obtained for the Richardson algorithm, Eq.(25). Thus the Liebmann algorithm converges just twice as fast as the Richardson algorithm--- that is, half as many iterations are necessary to obtain a given accuracy.

7. Liebmann Al gorithm; Two-dimensional Problem, Fixed boundary Conditions

This problem is discussed by Frankel. We shall briefly summarize the treatment. The mesh is the same as that considered in Section 2; but replacing Eq.(32) we now have

$$\epsilon_{ij}^{(n+1)} = \frac{1}{4}\left(\epsilon_{i-1,j}^{(n+1)} + \epsilon_{i,j-1}^{(n+1)} + \epsilon_{i+1,j}^{(n)} + \epsilon_{i,j+1}^{(n)}\right), \quad i=1,\dots,N_1-1;\ j=1,\dots,N_2-1, \tag{81}$$

$$\epsilon_{0j}^{(n)} = \epsilon_{N_1 j}^{(n)} = \epsilon_{i0}^{(n)} = \epsilon_{iN_2}^{(n)} = 0 \qquad \text{for all } n.$$

These equations can be written in the form

$$E^{(n+1)} = L E^{(n)} \tag{82}$$

but it is scarcely worth our while to give L explicitly. The eigenvalue problem for L can be obtained from Eqs.(81) by replacement of $\epsilon_{ij}^{(n+1)}$ by $\lambda \epsilon_{ij}^{(n)}$. The resulting equations are

$$0 = \lambda\{4x_{ij} - x_{i-1,j} - x_{i,j-1}\} - x_{i+1,j} - x_{i,j+1}, \quad i=1,\dots N_1-1,\ j=1\dots N_2-1, \tag{83}$$

$$x_{i0} = x_{iN_2} = x_{0j} = x_{N_1 j} = 0$$

On the basis of our experience with the one-dimensional problem, we make the following "guess" at the solution of Eqs.(83):

$$x_{ij} = A^{i+j} \sin i\theta_1 \sin j\theta_2,$$

$$\theta_1 = \frac{\pi}{N_1} r, \qquad \theta_2 = \frac{\pi}{N_2} s, \qquad r=1\dots N_1-1,\ s=1\dots N_2-1. \tag{84}$$

These solutions satisfy the boundary conditions of the problem. If Eq.(84) is substituted into Eqs.(83) one obtains after some simple algebra

$$0 = \{\lambda(4A - \cos\theta_1 - \cos\theta_2) - A^2(\cos\theta_1 + \cos\theta_2)\}\sin i\theta_1 \sin j\theta_2 + (\lambda - A^2)(\cos i\theta_1 \sin j\theta_2 \sin\theta_1 + \sin i\theta_1 \cos j\theta_2 \sin\theta_2). \tag{85}$$

The two terms of the right side of this equation must separately be zero (as can readily be shown by multiplication of the equations by

$\sin i\theta_1 \sin j\theta_2$ followed by summation over i and j). Hence

$$\lambda = A^2 \tag{86}$$

and

$$A = \frac{1}{2}(\cos\theta_1 + \cos\theta_2) \qquad \text{or} \qquad 0 \quad . \tag{87}$$

Let us count the number of independent eigenvectors that we have actually found in Eq. (84) . Note that according to Eq. (87) if we replace θ_1 by $\pi - \theta_1$ and θ_2 by $\pi - \theta_2$ then A changes sign though λ is unaffected. This same change in Eq. (84) leaves x_{ij} unchanged. Thus the solutions given by Eq. (84) do not, as may appear to be the case at first sight, form a complete set of eigenvectors. In order that these vectors be truly independent it is necessary to impose the additional condition

$$\theta_1 + \theta_2 \leq \pi \tag{88}$$

so that Eq. (84) yields about half the number of eigenvectors required for a complete set. These are, however, all the eigenvectors that L has. This statement can be verified by referral to Frankel's paper. Frankel considers a more general form of the algorithm involving a parameter α . Replacing Eq. (83) he has

$$\lambda x_{ij} = x_{ij} + \alpha\left(\lambda x_{i-1,j} + x_{i+1,j} + \lambda x_{i,j-1} + x_{i,j+1} - 4x_{ij}\right) \tag{89}$$

which reduces to Eq. (83) when $\alpha = \frac{1}{4}$. For α different from $\frac{1}{4}$ these equations yield a complete set of eigenvectors of the form of Eq. (84) belonging to distinct eigenvalues. As α approaches $\frac{1}{4}$ a number of the eigenvalues approach the value zero and their corresponding eigenvectors also approach zero. Those eigenvectors and eigenvalues that do not vanish in the limit of $\alpha = \frac{1}{4}$ are just the ones we have found. The situation is therefore identical with the one we faced in the one-dimensional case and the theorem proved in the Appendix applies.

The largest eigenvalue of L is

$$\lambda_{max} = \frac{1}{4}\left[\cos\frac{\pi}{N_1} + \cos\frac{\pi}{N_2}\right]^2 \simeq 1 - \frac{1}{2}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2\right] \tag{90}$$

and the lapse rate is

$$\mu \simeq \frac{1}{\ln 10}\,\frac{1}{2}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2\right], \tag{91}$$

just twice that obtained for the Richardson algorithm.

8. Liebmann Algorithm; Three-dimensional Problem: Fixed Boundary Conditions

The procedure is identical with that in the preceding section and yields the results

$$\lambda_{max} = \frac{1}{9}\left\{\cos\frac{\pi}{N_1} + \cos\frac{\pi}{N_2} + \cos\frac{\pi}{N_3}\right\}^2 \simeq 1 - \frac{1}{3}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right], \tag{92}$$

$$\mu \simeq \frac{1}{\ln 10}\cdot\frac{1}{3}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right] \tag{93}$$

where N_1+1, N_2+1, N_3+1 are the extents of the mesh (including the boundary points) in the i, j, k-directions respectively.

9. Liebmann Algorithm: Two-dimensional Problem: Periodic Boundary Conditions

The mesh and boundary conditions are described in Section 5. The effect of the periodic boundary conditions in the present case is much the same as with the Richardson Algorithm. The results of the calculation are

$$\lambda = \frac{1}{4}\left(\cos\theta_1 + \cos\theta_2\right)^2,$$
$$\theta_1 = \frac{2\pi}{N_1}r, \quad \theta_2 = \frac{\pi}{N_2}s, \qquad r = 0, \cdots, N_1-1;\ s = 1, \cdots, N_2-1, \tag{94}$$
$$\theta_1 + \theta_2 \leq \pi$$

so that

$$\lambda_{max} = \frac{1}{4}\left(1 + \cos\frac{\pi}{N_2}\right)^2 \simeq 1 - \frac{1}{2}\left(\frac{\pi}{N_2}\right)^2 , \tag{95}$$

and

$$\mu \simeq \frac{1}{\ln 10} \cdot \frac{1}{2}\left(\frac{\pi}{N_2}\right)^2 . \tag{96}$$

Once again the lapse rate is independent of the period of the mesh, N_1 .

10. Liebmann Algorithm: Three-dimensional Problem; Periodic Boundary Conditions

The problem is that stated in Section 5. For the mesh periodic in the i-direction we now have, replacing Eq. (52),

$$\mu \simeq \frac{1}{\ln 10} \cdot \frac{1}{3}\left[\left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right] , \tag{97}$$

while for the mesh periodic in the i- and j- directions one obtains

$$\mu \simeq \frac{1}{\ln 10} \; \frac{1}{3}\left(\frac{\pi}{N_3}\right)^2 . \tag{98}$$

11. Summary of Results

We present below the lapse rates for all cases discussed in this report employing the <u>Liebmann</u> algorithm. In all cases the Richardson algorithm yields lapse rates that are one-half those given in the table. In the cases referring to periodic boundary conditions it is the size of the mesh in the direction in which the periodicity occures that does not appear in the formulae.

No. of Dimensions	Boundary Conditions	Lapse rate in nepers/iteration
1		$\left(\frac{\pi}{N}\right)^2$
2	Fixed	$\frac{1}{2}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2\right]$
3	Fixed	$\frac{1}{3}\left[\left(\frac{\pi}{N_1}\right)^2 + \left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right]$
2	Periodic	$\frac{1}{2}\left(\frac{\pi}{N_2}\right)^2$
3	Periodic in one direction	$\frac{1}{3}\left[\left(\frac{\pi}{N_2}\right)^2 + \left(\frac{\pi}{N_3}\right)^2\right]$
3	Periodic in two directions	$\frac{1}{3}\left(\frac{\pi}{N_3}\right)^2$

12. Machine time for a Three-Dimensional Problem

The error in the potential at some particular checkpoint in the mesh is, after n iterations (where n is large), given by

$$\epsilon^{(n)} = \lambda_{max}^{n} \epsilon_0 \simeq 10^{-\mu n} \epsilon_0$$

where ϵ_0 is the initial error. The computation is considered finished when the change in the potential at the checkpoint between successive iterations becomes smaller than some preassigned value Δ (called ϵ on the agenda sheets for Forocyl). If I is the number of iterations required for the solution of a problem then

$$\frac{\Delta}{\epsilon_0} = \frac{\epsilon_I - \epsilon_{I+1}}{\epsilon_0} = \lambda^I (1-\lambda) \simeq \mu \ln 10 \cdot 10^{-\mu I}$$

so that

$$I = \frac{1}{\mu} \log \left(\frac{\epsilon_0 \mu \ln 10}{\Delta} \right) ,$$

which, except for notation, is the equation given in report MURA-251.

Let us consider the case most likely to arise in MURA work, that of a three-dimensional mesh with periodicity in one direction. If we take $N_1 = N_2 = N_3 = N$ the lapse rate (for the Liebmann algorithm) is given by

$$\mu \simeq \frac{1}{\ln 10} \cdot \frac{2}{3} \left(\frac{\pi}{N} \right)^2$$

so that

$$I = \frac{3}{2} (\ln 10) \left(\frac{N}{\pi} \right)^2 \log \left(\frac{2}{3} \left(\frac{\pi}{N} \right)^2 \frac{\epsilon_0}{\Delta} \right) .$$

We can put some resonable numbers into this formula. Since the IBM 704 can accomodate about 6000 mesh points (in a calculation in which the potentials alone are sought and not the fields) we can take $N = 18$. Let $\Delta = 10^{-10}$ and $\epsilon_0 = 10^{-2}$. Then the formula above gives

as $I \simeq 720$ iterations. The time needed by the computer for each point in the mesh in each iteration is of the order of .5 msec, so that in this example the total time needed for the problem is of the order of $T \simeq \left(.5\times10^{-3}\ \frac{\text{sec.}}{\text{point}\cdot\text{iteration}}\right)\cdot\left(6000\text{ points}\right)\left(720\text{ iterations}\right)=2160$ sec. or about 36 minutes which is not an unreasonable demand of machine time.

Appendix I

Remarks on Problems in Which the Normal Derivative of the Potential is Given

We consider the rectangular mesh of points shown in the figure. The potential is specified along the sides $j=0$ and $j=M_2$, the normal derivative of the potential, $\frac{\partial V}{\partial y}$, is specified along the sides $i=0$ and $i=M_1$. It is desired to solve Laplace's Equation subject to these boundary conditions.

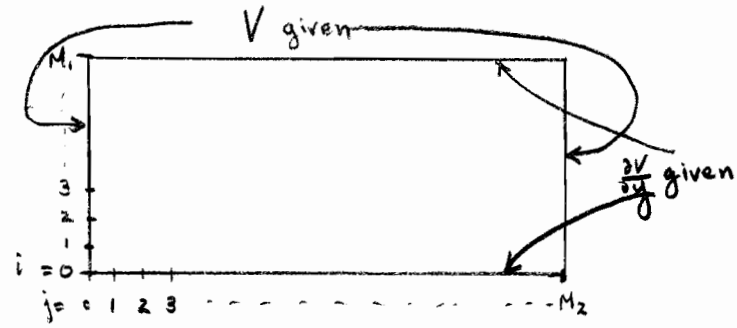

Fig. A1

The above is an instance of the type of computational problem met up with at Los Alamos. The authors do not know exactly what algorithm was used at Los Alamos but we assume for simplicity that the Richardson algorithm was used, so that for the interior points of the mesh the calculated potential on the $(n+1)$-st. iteration are given by

$$\varphi_{ij}^{(n+1)} = \frac{1}{4}\left(\varphi_{i-1,j}^{(n)} + \varphi_{i,j-1}^{(n)} + \varphi_{i+1,j}^{(n)} + \varphi_{i,j+1}^{(n)}\right), \tag{I.1}$$

$$i = 1,2, \ldots, M_1-1 \; ; \quad j = 1,2, \ldots, M_2-1 \; .$$

We can derive an algorithm for the points on the boundary $i=0$ as follows. Let V_{0j} be the potential at the point $(0,j)$, $(V_{0j})_x$ and $(V_{0j})_y$ its first derivatives at that point, and so on for higher derivatives. The potential at neighboring points can be obtained by a Taylor expansion of the potential in the neighborhood of point $(0,j)$, so that

$$V_{0\,j-1} = V_{0j} - (V_{0j})_x + \tfrac{1}{2}(V_{0j})_{xx} + \cdots \; ,$$

$$V_{0\,j+1} = V_{0j} + (V_{0j})_x + \tfrac{1}{2}(V_{0j})_{xx} + \cdots \; , \tag{I.2}$$

$$V_{1,j} = V_{0j} + (V_{0j})_y + \tfrac{1}{2}(V_{0j})_{yy} + \cdots \; .$$

Then by using the fact that V satisfies Laplace's equation, so that

$$(V_{0j})_{xx} + (V_{0j})_{yy} = 0 \quad ,$$

we obtain

$$V_{0j-1} + V_{0j+1} + 2V_{1,j} = 4V_{0j} + 2(V_{0j})_y + \cdots \tag{I.3}$$

Thus the algorithm for the boundary points in question should be

$$\varphi_{0j}^{(n+1)} = \frac{1}{4}\left(\varphi_{0j-1} + \varphi_{0j+1} + 2\varphi_{1,j}\right) - \frac{1}{2}(V_{0j})_y \tag{I.4}$$

where $(V_{0j})_y$ is given. In a similar fashion one obtains for the points on the boundary $i = M_1$

$$\varphi_{M_1,j}^{(n+1)} = \frac{1}{4}\left(\varphi_{M_1,j-1} + \varphi_{M_1,j+1} + 2\varphi_{M_1-1,j}\right) + \frac{1}{2}(V_{M_1,j})_y . \tag{I.5}$$

If one now considers the errors, that is the deviations of the calculated potentials, $\varphi_{ij}^{(n)}$, from the limiting potentials obtained from the algorithm, ϕ_{ij}, one obtains

$$\begin{aligned}
\epsilon_{ij}^{(n+1)} &= \frac{1}{4}\left(\epsilon_{i-1,j}^{(n)} + \epsilon_{i,j-1}^{(n)} + \epsilon_{i+1,j}^{(n)} + \epsilon_{i,j+1}^{(n)}\right) , \quad i = 1, \cdots M_1-1 ; \quad j = 1, \cdots M_2-1 , \\
\epsilon_{0j}^{(n+1)} &= \frac{1}{4}\left(\epsilon_{0j-1}^{(n)} + \epsilon_{0j+1}^{(n)} + 2\epsilon_{1,j}^{(n)}\right) , \quad j = 1, \cdots, M_2-1 \\
\epsilon_{M_1,j}^{(n+1)} &= \frac{1}{4}\left(\epsilon_{M_1,j-1}^{(n)} + \epsilon_{M_1,j+1}^{(n)} + 2\epsilon_{M_1-1,j}^{(n)}\right) , \quad j = 1, \cdots, M_2-1 ,
\end{aligned} \tag{I.6}$$

$$\epsilon_{i0} = \epsilon_{iM_2} = 0$$

or

$$E^{(n+1)} = K E^{(n)} \tag{I.7}$$

where K is a square matrix with $(M_1+1)(M_2-1)$ rows. The lapse rate is determined by the largest eigenvalue of the matrix K.

The eigenvalue problem for K can be solved by reduction of the problem to the one already solved in section 4. Consider the mesh shown in the figure.

This mesh is obtained by reflection of the mesh in Figure A1 in the line $i=0$. The potentials at the points along the boundaries $j=0$ and $j=M_2$ with $i \geq 0$ are the same as those specified in the original mesh while the potentials at $j=0$ and $j=M_2$ with $i<0$ are obtained by reflection in $i=0$. For this new problem we assume peroidicity of the potential along the direction of increasing i with peroid $2M_1$. The equations describing the errors in the calculated potential for this problem are given by Eqs. (44) with N_2 replaced by M_2 and i assuming integral values from $-M_1$ to $+M_1$. If we seek only those solutions that posess mirror symmetry about the line $i=0$, that is, if we put

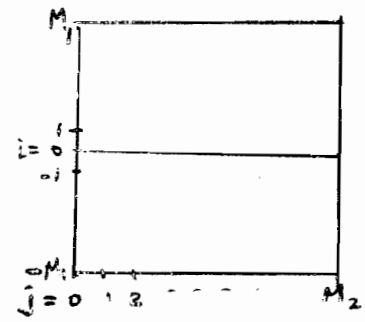

Figure A2

$$\epsilon^{(m)}_{-ij} = \epsilon^{(m)}_{ij} \tag{I.8}$$

then these equations become identical with Eqs. (I.6) except for repetitions. Hence the eigenvectors of K are just the first M_1+1 components of those eigenvectors of L for the periodic problem possessing mirror symmetry around the component $i=0$. The eigenvalues of K are the same as the eigenvalues of L corresponding to these symmetric eigenvectors. These eigenvectors of L are given by Eq. (47), that is,

$$x_{ij} = \left(\cos i\frac{\pi}{2M_1} r\right)\left(\cos j\frac{\pi}{M_2} s\right),$$
$$r = 0, 2, \cdots, 2M_1; \quad s = 1, 2, \cdots, M_2-1, \tag{I.9}$$

and the corresponding eigenvalues are

$$\lambda = \frac{1}{2}\left(\cos\frac{\pi}{2M_1} r + \cos\frac{\pi}{M_2} s\right). \tag{I.10}$$

The eigenvalue of largest magnitude is

$$\lambda_{max} = \frac{1}{2}\left(1+\cos\frac{\pi}{M_2}\right) \cong 1 - \frac{1}{4}\left(\frac{\pi}{M_2}\right)^2 \tag{I.11}$$

and the lapse rate in decades per iteration is

$$\mu \cong \frac{1}{\ln 10} \cdot \frac{1}{4}\left(\frac{\pi}{M_2}\right)^2 \tag{I.12}$$

independent of M_1. For a mesh of given size, therefore, there is a considerable difference between the lapse rates for a case in which the potential is specified along the shorter side of the rectangle and the case in which the potential is specified along the longer side of the rectangle, as was observed at Los Alamos.

The treatment above assumed the use of the Richardson algorithm but this assumption is irrelevant to the main point----the same effect results from the use of the Liebmann algorithm.

This same kind of argument can be used to obtain the lapse rates for a variety of other problems. Consider, for example, the mesh shown in Figure A3. The lapse rate for this problem is the same as that for the mesh shown in Fig. A2 with the following boundary conditions applied: the potential is periodic in the x -direction with period M_2, it is periodic in the y -direction with period $2M_1$ and is specified along the line $i=0$. If the Richardson algorithm is used with these boundary conditions then the equations satisfied by the ϵ's are

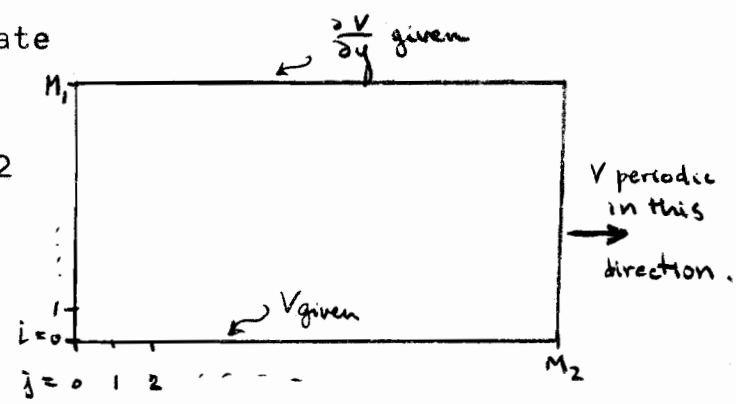

Fig. A3

$$\epsilon_{ij}^{(n+1)} = \frac{1}{4}\left(\epsilon_{i-1,j}^{(n)} + \epsilon_{i,j-1}^{(n)} + \epsilon_{i+1,j}^{(n)} + \epsilon_{i,j+1}^{(n)}\right), \quad \left.\begin{array}{l} i=-M_1+1,\ldots,-1,0,1,\ldots,M_1, \\ j=1,\ldots,M_2 \end{array}\right\} \tag{I.13}$$

$$\epsilon_{i+2M_1,j}^{(n)} = \epsilon_{ij}^{(n)}; \quad \epsilon_{i,j+M_2}^{(n)} = \epsilon_{ij}^{(n)}; \quad \epsilon_{0j}^{(n)} = 0 .$$

Except for the boundary conditions one can readily see that these equations are the same as Eqs. (44) . It is clear that the eigenvectors of the corresponding matrix (with these boundary conditions) are

$$x_{ij} = \sin i\theta_1 \begin{cases} \sin j\theta_2 \\ \cos j\theta_2 \end{cases} ,$$

$$\theta_1 = \frac{2\pi}{2M_1} r \quad , \quad r = 1, \cdots, 2M_1 - 1 , \tag{I.14}$$

$$\theta_2 = \frac{\pi}{M_2} s \quad , \quad s = 0, 2, 4, \cdots, \begin{cases} M_2 \text{ if } M_2 \text{ is even} \\ M_2 - 1 \text{ if } M_2 \text{ is odd} \end{cases} ,$$

the corresponding eigenvalues being

$$\lambda = \frac{1}{2}(\cos\theta_1 + \cos\theta_2) .$$

The largest eigenvalue is

$$\lambda_{max} = \frac{1}{2}\left(1 + \cos\frac{\pi}{2M_1}\right) \cong 1 - \frac{1}{4}\left(\frac{\pi}{2M_1}\right)^2 \tag{I.15}$$

and the lapse rate is therefore

$$\mu \simeq \frac{1}{\ln 10} \cdot \frac{1}{4}\left(\frac{\pi}{2M_1}\right)^2 \tag{I.16}$$

which is just one-quarter of the lapse rate for the problem in which V is given on both horizontal surfaces in Fig. A3. The same kind of result obtains if the Liebmann algorithm is used, the lapse rate for the Liebmann algorithm being twice that [redacted] for the Richardson algorithm.

Appendix II

Proof of the Theorem Stated in Section 6

Denote the linear manifold spanned by $X_1, \ldots, X_r$ by M_1. Let M_2 be the manifold orthogonal to M_1, so that the entire vector space is the Cartesian sum of M_1 and M_2. Let $Y_1, \ldots Y_r$ be an orthogonal basis for M_1 and $Y_{r+1}, \ldots, Y_n$ an orthogonal basis for M_2. Decompose the operator T as follows:

$$T = T_1 + T_2 + T_3$$

where

T_1 transforms a vector in M_1 into a vector in M_1,

T_2 transforms a vector in M_2 into a vector in M_1,

T_3 transforms a vector in M_2 into a vector in M_2.

Such a decomposition is always possible since M_1 is an invariant manifold of T (any linear combination of eigenvectors is transformed by T into a linear combination of eigenvectors).

T_1 by itself, as an operator in an r-dimensional space, has eigenvalues $\lambda_1, \ldots, \lambda_r$. In a representation with the Y's as basis vectors the matrix T is

$$\left(\begin{array}{c|c} T_1 & T_2 \\ \hline 0 & T_3 \end{array}\right) \begin{array}{l} \left.\vphantom{\begin{array}{c}T\\T\end{array}}\right\} r \text{ rows} \\ \left.\vphantom{\begin{array}{c}T\\T\end{array}}\right\} n-r \text{ rows} \end{array}$$

and the secular equation of T becomes

$$0 = \left|\begin{array}{c|c} T_1 - \lambda 1 & T_2 \\ \hline 0 & T_3 - \lambda 1 \end{array}\right| = |T_1 - \lambda 1| \cdot |T_3 - \lambda 1|$$

The factor $|T_1-\lambda 1|$ provides the roots $\lambda_1, \cdots, \lambda_r$. The factor $|T_3-\lambda 1|$ must provide the remaining roots of the secular equation for T, all of which are zero. Hence the secular equation of T_3 is

$$|T_3 - \lambda 1| = \text{constant} \times \lambda^{n-r} = 0 .$$

According to the Cayley-Hamilton theorem, T_3 satisfies its own secular equation, so that

$$T_3^{n-r} = 0 .$$

Now consider T^{n-r} with the Y's as a basis. It has the form

$$T^{n-r} = \left[\begin{array}{c|c} T_1^{n-r} & P \\ \hline & T_3^{n-r} \end{array}\right] = \left[\begin{array}{c|c} T_1^{n-r} & P \\ \hline & 0 \end{array}\right]$$

where P is some polynomial in T_1, T_2, T_3. Hence if Z is an arbitrary linear combinatioin of $Y_{r+1}, \cdots, Y_n$, that is, in the Y-representation the first r components of Z are zero, then

$$T^{n-r} Z = 0 .$$