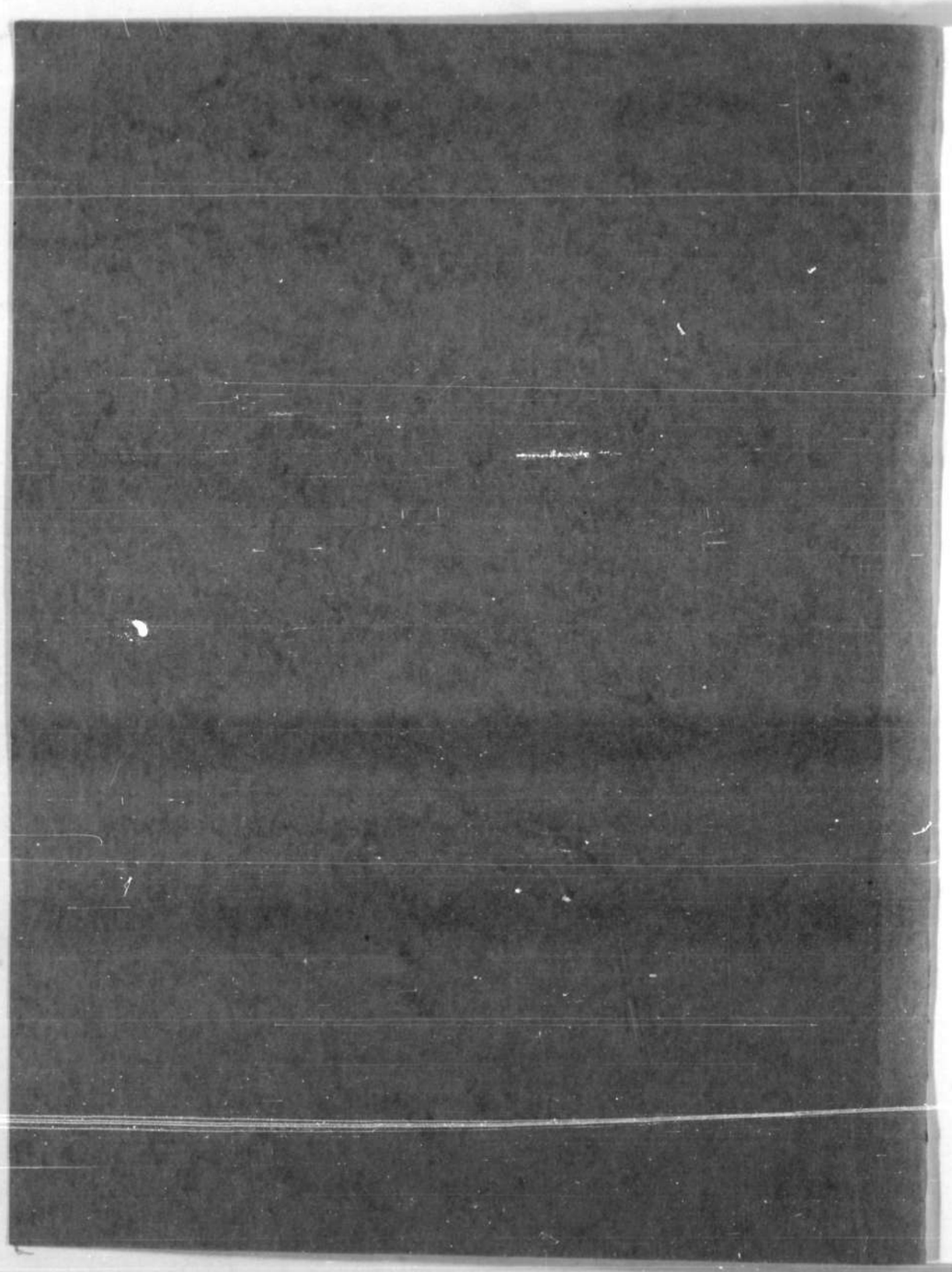

MACHINE METHODS OF COMPUTATION

and

NUMERICAL ANALYSIS

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PROJECT WHIRLWIND

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FOREWORD

This is a combined report for the two projects at the Massachusetts Institute of Technology which are sponsored by the Office of Naval Research under Contract N5or160.

Project on Machine Methods of Computation and Numerical Analysis

This Project is an outgrowth of the activities of the Institute Committee on Machine Methods of Computation, established in November 1950. The purpose of the Project is (1) to integrate the efforts of all the departments and groups at M.I.T. who are working with modern computing machines and their applications, and (2) to train men in the use of these machines for computation and numerical analysis.

People from several departments of the Institute are taking part in the project. In the Appendix will be found a list of the personnel active in this program.

Project Whirlwind

This Project makes use of the facilities of the Digital Computer Laboratory. The principal objective of the Project is the application of an electronic digital computer of large capacity and very high speed (Whirlwind I) to problems in mathematics, science, engineering, simulation, and control.

The Whirlwind I Computer

Whirlwind I is of the high-speed electronic digital type, in which quantities are represented as discrete numbers, and complex problems are solved by the repeated use of fundamental arithmetic and logical (i.e., control or selection) operations. Computations are executed by fractional-microsecond pulses in electronic circuits, of which the principal ones are (1) the flip-flop, a circuit containing two vacuum tubes so connected that one tube or the other is conducting, but not both; (2) the gate or coincidence circuit; (3) the magnetic-core memory, in which binary digits are stored as one of two directions of magnetic flux within ferro-magnetic cores.

Whirlwind I uses numbers of 16 binary digits (equivalent to about 5 decimal digits). This length was selected to limit the machine to a practical size, but it permits the computation of many simulation problems. Calculations requiring greater number length are handled by the use of multiple-length numbers. Rapid-access magnetic-core memory has a capacity of 32,768 binary digits. Present speed of the computer is 40,000 single-address operations per second, equivalent to about 20,000 multiplications per second.

PART I

Machine Methods of Computation and Numerical Analysis

1. GENERAL COMMENTS

During the quarter reported here, integration of the work of the Project with the general research of the Institute has proceeded apace. Whirlwind I has been used by a wider variety of research projects and the Machine Methods and Numerical Analysis staff have helped translate a wider variety of computational problems into machine language than previously. One new area of note is in the difficult field of weather forecasting. The Project sponsored a series of seminars where some of the basic problems were discussed by members of the Meteorology Department and by Professor Norbert Wiener. The report entitled "Multiple Prediction Theory" outlines the resulting work to date.

The research projects reported in the following pages represent a wide variety of subjects; their common aspects lie in the adaptation of the problem for machine computation. Each application has added to our experience in the techniques of such application; many of them have resulted in useful sub-routines, which are now in the Whirlwind library, available to other workers.

2. GRADUATE SCHOOL RESEARCH

2.1 Index to Reports

2.2 Progress Reports

MULTIPLE PREDICTION THEORY

During the last quarter some work on prediction theory was begun and completed. This work was stimulated by two of the project seminars in which the application, computation, and theory of prediction was presented by Professor Thomas F. Malone and Mr. Robert G. Miller of the Meteorology Department and Professor Norbert Wiener of the Mathematics Department. The seminars and the ensuing discussions will be reported more completely in the Section 3 on Academic Program. The work outlined in this report was done in collaboration with Professor Wiener and will be presented in detail in one of the mathematics journals.

The theory of the best linear prediction of a single stationary time series was developed simultaneously in Russia and the United States about fifteen years ago [1, 2]. The men chiefly responsible for this work were A. Kolmogorov and Norbert Wiener. The essential foundations for the prediction of more than one time series has only recently been made available and this is to be found in Professor Wiener's matrix factorization work [3]. Most of the results reported here are essentially the matrix factorization expressed in the explicit language of prediction theory.

Suppose that two simultaneous series of measurements are made at integer points in time and suppose that these two series are the measured values of two parameters, respectively, belonging to the same physical system. Thus, as time progresses and a dynamics carries the physical system from state to state, the measured values of two of the parameters of the system will change. It is the job of the mathematician to predict the value of either or both of these parameters at some specified time in the future, given a knowledge of their past history up to and including the present. It is, of course, impossible to do this prediction precisely and under all circumstances, and thus it is also the job of the mathematician to set down those criteria for a good prediction and those conditions under which prediction becomes possible with our present state of knowledge. It will turn out that the conditions are also justified in most cases where we desire to put prediction into practice.

The state of the system at any particular time, say the present, is assumed to be a random variable and, without loss of generality, is assumed to be a uniformly distributed random variable taking values on the interval $[0, 1]$. This variable will be denoted by "α." It is also assumed that the system is conservative so that the dynamics which carry the system from one state, α, at time zero, to another state, α', at one unit in the future can be represented as a measure-preserving point transformation, T, that possesses an inverse and is such that $T(\alpha) = \alpha'$. In general, during n-units of time the dynamics will carry the point α into the point $T^n(\alpha)$.

Now let f_1 and f_2 be two parameters depending on the system so that at time n

$$f_1 = f_1(T^n\alpha), \quad f_2 = f_2(T^n\alpha).$$

If the series of values of the two parameters measured at time zero, one unit in the past, two units in the past, etc., are written:

$$f_1(\alpha),\ f_1(T^{-1}\alpha),\ f_1(T^{-2}\alpha),\ldots$$

$$f_2(\alpha),\ f_2(T^{-1}\alpha),\ f_2(T^{-2}\alpha),\ldots$$

Then a "good" linear prediction of the value $f_1(T^m\alpha)$; $i = 1, 2$; $m > 0$ will be that linear combination

$$L_1^{(m)}(\alpha) = \sum_{j=1,2} \sum_{n=0}^{\infty} f_j(T^{-n}\alpha) P_n^{(m)}(i, j)$$

such that

$$(1) \qquad \int_0^1 \left[f_1(T^m\alpha) - L_1^{(m)}(\alpha)\right]^2 d\alpha$$

is a minimum. The minimum value of expression (1) is the mean-square-error for the indicated prediction, where the averaging is taken over the ensemble of all possible states of the system. The criterion for "goodness" identifies as a solution to the prediction problem that linear combination whose mean-square-error is least.

The assumption that T is measure-preserving is equivalent to the assumption that both time series are stationary and helps make the following solution possible. A second assumption that must be made for the following solution is equivalent to asking that the time

series do not contain any deterministic components; that is, any components which could be predicted with zero mean-square-error.

With these assumptions Professor Wiener has shown [3] that it is possible to expand either function $f_i(\alpha)$, $i = 1, 2$, in terms of an orthogonal set

$$q_j(T^{-n}\alpha)\ ,\ j = 1, 2,\ n = 0, 1, 2, \ldots,$$

$$(q_i, q_j T^{-n}) = \int_0^1 q_i(\alpha)\overline{q_j(T^{-n}\alpha)}\,d\alpha = \begin{cases} 1 & n = 0,\ i = j \\ 0 & \text{Otherwise,} \end{cases}$$

where $q_j(\alpha)$ is linearly dependent on $f_1(\alpha)$, $f_2(\alpha)$, $f_1(T^{-1}\alpha)$, $f_2(T^{-1}\alpha)$, $f_1(T^{-2}\alpha)$, $f_2(T^{-2}\alpha)$, ... Thus:

$$(2) \qquad f_i(\alpha) = \sum_{j=1,2} \sum_{n=0}^{\infty} q_j(T^{-n}\alpha)(f_i, q_j T^{-n}).$$

In other words, if $m > 0$,

$$(3) \qquad f_i(T^m\alpha) = F_i^{(m)}(\alpha) + G_i^{(m)}(\alpha)$$

$$= \sum_{j=1,2} \sum_{n=m}^{\infty} q_j(T^{m-n}\alpha)(f_i, q_j T^{-n})$$

$$= \sum_{j=1,2} \sum_{n=0}^{m-} q_j(T^{m-n}\alpha)(f_i, q_j T^{-n}).$$

where $F_i^{(m)}(\alpha)$ is linearly dependent on the present and the past of both time series and

$$f_i(T^m\alpha) - F_i^{(m)}(\alpha) = G_i^{(m)}(\alpha)$$

is orthogonal to the present and past of both series. This, however, is equivalent to saying that $F_i^{(m)}(\alpha)$ is the best linear prediction of $f_i(T^m\alpha)$ in the sense defined above. If we use the fact that

$$(4) \qquad q_i(\alpha) = \sum_{j=1,2} \sum_{n=0}^{\infty} f_j(T^{-n}\alpha)\ell_n(i, j)$$

for some coefficients $\ell_n(i, j)$, a little computation immediately shows that

$$(5) \qquad F_i^{(m)}(\alpha) = \sum_{j=1,2} \sum_{n=0}^{\infty} f_j(T^{-n}\alpha) \sum_{\mu=0}^{n} \left\{ \sum_{j=1,2} \ell_{n-\mu}(j, j)\varphi_{\mu+m}(i, j) \right\},$$

where $\varphi_{\mu+m}(i, j) = (f_i, q_j T^{-m-\mu})$. The coefficients $P_n^{(m)}(i, j)$ in the best linear prediction of $f_i(T^m\alpha)$ are found to be:

$$(6) \qquad P_n^{(m)}(i, j) = \sum_{\mu=0}^{n} \left\{ \sum_{j=1,2} \ell_{n-\mu}(j, j)\varphi_{\mu+m}(i, j) \right\}.$$

The coefficients $\ell_n(i, j)$ are immediately found in terms of $\varphi_n(i, j)$ from (4) and the orthogonality relations of $q_i(T^n\alpha)$. It remains to determine $\varphi_n(i, j)$ from some measurable quantities.

Some direct calculations from Wiener's series expressions for $q_j(\alpha)$ give $\varphi_n(i, j)$ in series form with the terms of the series involving

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\Phi_{ij}(\theta)}{\Psi_i(\theta)\overline{\Psi_j(\theta)}}\, e^{-in\theta}d\theta$$

and

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \Psi_i(\theta)e^{-in\theta}d\theta,$$

where $\Psi_i(\theta)$ has the property that it can be determined, as in the one series case, from its

absolute squared value. The last two sets of quantities can be shown to be related to the auto and cross-correlations of the original series in the following way:

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \Phi_{ij}(\theta)e^{-in\theta}d\theta = (f_i T^n, f_j)$$

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} |\Psi_i(\theta)|^2 e^{-in\theta}d\theta = (f_i T^{-n}, f_i).$$

Finally, if we assume that T is ergodic, these auto and cross-correlations can be computed solely with a knowledge of the present and the past of the original time series:

$$(7) \qquad (f_i T^{-n}, f_j) = \lim_{N\to\infty} \frac{1}{N+1} \sum_{\mu=0}^{N} f_i(T^{-\mu}\alpha)\overline{f_j(T^{-n-\mu}\alpha)}.$$

The solution for the prediction of three and more time series generalizes immediately from the above results.

Bayard Rankin

References:

[1] Norbert Wiener, Extrapolation, Interpolation, and Smoothing of Stationary Time Series, The Technology Press of M.I.T. and John Wiley and Sons, Inc., New York (1949).

[2] A. N. Kolmogorov, Bull. Acad. Sci. URSS, Ser. Math. 5 (1941) pp. 3-14.

[3] Norbert Wiener, Commentarii Mathematici Helvetici, 29 (1955) pp. 97-111.

COUNTING STRUCTURES OF FINITE RELATIONS

A Whirlwind I program for counting dyadic relations on a finite set has been written and tested [1]. The computations should be completed shortly.

Besides counting simply all the non-isomorphic structures of pairwise relations between objects of a set, formulas are also being evaluated for the numbers of non-isomorphic structures in the following categories:

1. Reflexive relations. If the relation is specified in matrix form, $a_{ij} = 0, 1$ depending on whether element i of the set bears the relationship to element j, the reflexive relation has 1's on the diagonal. By writing 0's for 1's, a reflexive relation becomes irreflexive, which may be interpreted as the number of directed graphs (with at most one arrow $p_i \to p_j$) on n nodes $p_1, \ldots p_n$.

2. Symmetric relations: $a_{ij} = a_{ji}$.

3. Symmetric and irreflexive relations: $a_{ij} = a_{ji}$, $a_{ii} = 0$. This formula gives the number of non-directed graphs on n nodes with at most one connection $p_i \leftrightarrow p_j$.

4. Assymetric or antisymmetric relations: Here $a_{ij} = 1$ implies $a_{ji} = 0$, but a pair $a_{ij} = a_{ji} = 0$ is admissible. For assymetric relations $a_{ii} = 1$, for antisymmetric, $a_{ii} = 0$. These formulas are given by Davis [2].

References:

[1] Machine Methods of Computation and Numerical Analysis, Quarterly Progress Report No. 15, p. 10, March (1955).

[2] R. L. Davis, Proc. Am. Math. Soc. 4, 486 (1953).

M. Douglas McIlroy

MULTIPLE SCATTERING OF WAVES FROM A SPATIAL ARRAY OF SPHERICAL SCATTERERS

General Formulation - The task of devising an electronic wave function in a periodic lattice is primarily that of joining smoothly a central-force solution, appropriate for the almost spherically-symmetric atomic interiors, to a plane-wave solution, appropriate for the almost force-free interatomic regions. The work of Slater [1], Korringa [2], and others [3] indicates that whenever it is allowable to simplify the problem by saying that inside a sphere of radius a the effective potential is spherically symmetric and outside this sphere, out to the lattice cell boundaries, the effective potential is zero, then a technique of joining at the spherical surfaces r = a will produce the appropriate solution. Several forms of joining solutions can be derived; the important thing is to find a form which can be easily manipulated for calculation. The present paper discusses a modification of the forms given earlier, which appears quite promising.

To assume that the effective potential is spherically symmetric inside the sphere r = a and is zero in the interspaces is to make the problem identical with the acoustical problem of the transmission of sound waves through a regular array of spherical scatterers. In both cases we need not know the details of the wave solution inside the spheres in order to determine the solution in the interspace; all that is needed is the value of the logarithmic derivatives, at the surface r = a, of the interior radial factors for each spherical harmonic. In other words, if the wave function at the surface r = a is

$$(1) \qquad \Psi_{int} = \sum_{m\ell} F_{m\ell} Y_\ell^m(\vartheta,\varphi) \qquad (r = a)$$

where Y_ℓ^m are the usual spherical harmonics 4,then all we need to know about the interior, r < a, are the values of the various g's, defined in the equation

$$(2) \qquad (\partial\Psi_{int}/\partial r) = -(1/a)\sum_{m\ell} g_\ell F_{m\ell} Y_\ell^m \qquad (r = a)$$

Knowing values of the g's, the problem is essentially one of finding allowed values of the F's for the required lattice of spheres, subject to the requirement that, as one goes from the zero'th cell to the p'th cell in the lattice, the wave is multiplied by the factor $\exp(i\underline{K}.\underline{R}_p)$, where $\underline{K}$ is the wave number vector characterizing the particular solution and $\underline{R}_p$ is the displacement vector from the zero'th to the p'th cell. Knowing the F's it is, of course, easy then to find the wave solution inside the spheres, if this is needed. Equation (2) is also the appropriate form for acoustical waves in a lattice of spherical scatterers; in the acoustical case the g's may be complex numbers.

The solution in the field-free interspace can, of course, be expressed in terms of plane waves

$$(3) \qquad \Psi(\underline{r}) = \sum_\nu B_\nu \exp\left[i(\underline{K}_\nu+\underline{K}).\underline{r}\right] \qquad \text{(outside spheres)}$$

where $\underline{K}_\nu$ is the vector from the origin to the ν'th point in the reciprocal lattice, and the joining equations can be set up in terms of the B's instead of the F's. However, in actual practice series (3) converges much more slowly than series (1) so it is usually better to solve first for the F's, then for the B's.

The equation for the F's in terms of the g's is most easily obtained by use of the Green's function appropriate for the lattice, corresponding to a point source in each cell, at the point $\underline{r}_o + \underline{R}_p$, the source in the zero'th cell having unit amplitude and that in the p'th cell having amplitude $\exp(i\underline{K}.\underline{R}_p)$:

$$(4) \qquad G_{\underline{K},k}(\underline{r}\,|\,\underline{r}_o) = \sum_p \left[\exp(i\underline{K}.\underline{R}_p + ik|\underline{r}-\underline{r}_o-\underline{R}_p|)\right]/|\underline{r}-\underline{r}_o-\underline{R}_p|$$

$$= (4\pi/v)\sum_\nu \left[\exp\, i(\underline{K}_\nu+\underline{K}).(\underline{r}-\underline{r}_o)\right] / \left[|\underline{K}+\underline{K}_\nu|^2-k^2\right]$$

where v is the volume of one cell. These are, of course, conditionally convergent series; justification for their use will lie in the convergence of the integrals involving them.

The parameter k measures the energy of the electron or the frequency of the sound wave, since we assume that in the field-free interspace the homogeneous equation for Ψ or G is $\nabla^2\Psi + k^2\Psi = 0$. The joining equations for r = a must, of course, give us the relationship between $\underline{K}$ and k, in addition to determining the F's.

The integral equation for Ψ in the interspace between spheres is

$$\Psi(\underline{r}) = (1/4\pi)\int\left[G_{\underline{K}k}(\underline{r}\,|\,\underline{r}_s)(\partial\Psi/\partial n_s) - \Psi(\underline{r}_s)(\partial G_{\underline{K}k}/\partial n_s)\right] dS$$

over the central spherical surface and over the cell surface. Because of the periodicity of the product $G\Psi$, the integral over the cell surface vanishes so that outside r = a and on the surface

$$(5) \qquad \Psi(\underline{r}) = (a^2/4\pi)\int\left[\Psi(\underline{a}_o)(\partial G_{\underline{K}k}/\partial a_o) - G_{\underline{K}k}(\underline{r}\,|\,\underline{a}_o)(\partial\Psi/\partial a_o)\right] d\Omega_o$$

where $d\Omega_o$ is the element of solid angle $\sin\vartheta_o\, d\vartheta_o\, d\varphi_o$ and $\underline{a}_o$ is of length a, of direction given by ϑ_o,φ_o. Setting $\underline{r} = \underline{a}$ leads to an integral equation for Ψ on the surface of the sphere, which is the equation we desire. Using Equations (1) and (2), we obtain

$$(6) \qquad F_{m\ell} = a\sum_{m'\ell'} \frac{2\ell+1}{16\pi^2}\frac{(\ell-m)!}{(\ell+m)!}\iint \bar{Y}_\ell^m(\vartheta,\varphi)\left[g_\ell\, G_{\underline{K}k}(\underline{a}\,|\,\underline{a}_o)\right.$$

$$\left. + a(\partial G_{\underline{K}k}/\partial a_o)\right] Y_\ell^{m'}(\vartheta_o,\varphi_o)\, d\Omega\, d\Omega_o \Big\} F_{m'\ell'}$$

which is the fundamental homogeneous equation determining the F's and k in terms of $\underline{K}$.

Since Equation (6) is a homogeneous integral equation, it has non-zero solutions for only certain discrete values of k for a given $\underline{K}$. These are the allowed levels we seek. We can find this relationship by a variational method, as Kohn and Rostoker [3] suggest, or else we can solve the implicit set of simultaneous Equations (6) directly for k, for any chosen $\underline{K}$, since the $F_{m\ell}$'s converge quite rapidly.

To put Equation (6) in useable form, we apply the usual [3, 4] expansion of the Green's function (for $a < r < R_p$)

$$G_{\underline{K}k}(\underline{r}\,|\,\underline{a}_o) = .(ik/4\pi)\sum_p e^{i\underline{K}.\underline{R}_p}\int_B e^{i\underline{k}.(\underline{a}_o+\underline{R}_p-\underline{r})} d\Omega_k$$

$$= ik\sum_{m\ell}(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}\, Y_\ell^m(\vartheta,\varphi)\left\{\bar{Y}_\ell^m(\vartheta_o,\varphi_o)\right. \qquad J_\ell(ka)h_\ell(kr)$$

$$+ \sum_{m'\ell'} i^{\ell-\ell'}(2\ell'+1)\frac{(\ell'-m')!}{(\ell'+m')!}\,\bar{Y}_{\ell'}^{m'}(\vartheta_o,\varphi_o) J_{\ell'}(ka) J_\ell(kr).$$

$$\left.\sum_n i^n I_n(m\ell\,|\,m'\ell') \sum_{p\neq 0} Y_n^{m'-m}(\varrho_p,\varrho_p) e^{i\underline{K}.\underline{R}_p}\, h_n(kR_p)\right\}$$

where ϱ_p, ϱ_p are the spherical angles for the vector $\underline{R}_p$ and where the I's are the Gaunt factors, defined by the equations

$$(7) \qquad \bar{Y}_\ell^m(\vartheta,\varphi)Y_\ell^{m'}(\vartheta,\varphi) = \sum_n I_n(m\ell\,|\,m'\ell')Y_n^{m'-m}(\vartheta,\varphi)$$

We also need the g factors for the Spherical Bessel functions

$$(8) \qquad g_\ell^o(ka) = -\left[a/J_\ell(ka)\right]\left[dJ_\ell(ka)/da\right] = \tan\left[\alpha_\ell(ka)\right]$$

These would be the values of the g's for Equation (2) if the effective potential inside r = a were zero. Tables of α_ℓ are available [5].

Substituting all this in Equation (6) we obtain

$$(9) \qquad JF_{m\ell} = ka\, J_\ell(ka)\left\{i(g_\ell-g_\ell^o)h_\ell(ka)F_{m\ell}\right.$$

$$+ \sum_{m'\ell'} i^{\ell-\ell'}(g_\ell,-g_{\ell'}^o)J_{\ell'}(ka)\left[(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}\sum_n I_n(m\ell\ m'\ell')\cdot\right.$$

$$\left.\left.\sum_{p\neq 0} i^{n+1}Y_n^{m'-m}(\varrho_p,\varrho_p)e^{i\underline{K}.\underline{R}_p}\, n_n(kR_p)\right] F_{m'\ell'}\right.$$

where, for each choice of $\underline{K}$, k is adjusted to make J = 1. This is a compact and rapidly convergent form for use in computations. The quantities in square brackets do not depend on the spherical interiors and may be computed, once for all, for each type of lattice. The spherical interior only comes in with the terms $(g_\ell-g_{\ell'}^o)$, which are, as we shall see later, closely related to phase angles for scattering from a single sphere: These go rapidly to zero for increasing ℓ and in many cases only $\ell = 0,1,2$ suffice for three or four place computation of k and of the F's. The first-order effects of higher ℓ's may be added, if desired.

It will be shown later that for regular lattices the matrix of the coefficients of the F's is Hermitean as long as the g's are real, so the computed values of J are real when k and K are real. We will also show that when $k \to K$ the quantity in square brackets becomes inversely proportional to K^2-k^2, so that when the scatterer inside r = a is weak (or when $a \to 0$) and all the g's approach the g^0's, then k approaches K, as it should.

Furthermore, the Equations (9) are exact, as long as the initial assumptions (V = 0 for r > a) are valid. Although the derivation given above assumes a regular lattice, the same equation can be obtained without the assumption of regularity, as long as the mean density of spherical centers (i.e., the mean density of the points represented by the vectors $\underline{R}_p$) approaches a constant for large R. The summation over p is then the summation over all the other scattering centers, the p'th one being at $\underline{R}_p$. Effects of lattice distortion may thus be computed from the same equation.

From this point of view Equation (9) is an extension of the method of Foldy [6] for calculating the multiple scattering of sound from a random distribution of scatterers. The quantities in the square brackets represent the effect, on the surface of the central sphere, of the scattering from all the other spheres.

The Lattice Scattering Function - The basic lattice scattering functions [7] M^m_n are defined as follows:

$$i^{n+1} \sum_{p\neq 0} e^{i\underline{K}\cdot\underline{R}_p}\, Y^m_n(\vartheta_p,\phi_p) h_n(kR_p) = -i\delta_{om}\delta_{on} + M^m_n \tag{10}$$

It turns out that as k approaches K, M goes to infinity as $(4\pi/kv)(-K/k)^n Y^m_n(u_o, v_o)/(K^2-k^2)$, where v is the cell volume and u_o and v_o are the spherical angles for vector $\underline{K}$. In many parts of the calculations it is advisable to subtract it out. The functions M, as defined, are real quantities for regular lattices; they have a sequence of poles when $k^2 = |\underline{K}+\underline{K}_\nu|^2$ and except near the poles they are fairly well-behaved functions of k, having magnitudes of the order of unity.

The method of calculation of M is, of course, a generalization of the one used by Ewald [8], also by others [2, 3]. We substitute the source distribution

$$\rho(\beta) = i^{-n} \sum_{p\neq 0} (2^n \beta^{2n+3}/\pi^{\frac{1}{2}}\kappa^n) |\underline{r}-\underline{R}_p|^n\, Y^m_n(\vartheta_p,\phi_p) \cdot \exp\left[i\underline{K}\cdot\underline{R}_p + (\kappa/2\beta)^2 - \beta^2|\underline{r}-\underline{R}_p|^2\right]$$

(where ϑ_p, ϕ_p are the spherical angles for the vector $\underline{r}-\underline{R}_p$) instead of the set of point sources, $\rho(\infty)$, which produce the series on the left-hand side of Equation (10). Adding the term p = 0 to $\rho(\beta)$ allows the waves produced at the origin by this distribution to be expanded as a Fourier series, giving for part of M

$$M^o_{mn} = (-1)^n \frac{4\pi}{kv}\left\{\sum_\nu \left(\frac{|\underline{K}+\underline{K}_\nu|}{k}\right)^n \frac{\exp\left[-(1/4\beta^2)(|\underline{K}+\underline{K}_\nu|^2-k^2)\right]}{|\underline{K}+\underline{K}_\nu|^2 - k^2} Y^m_n(u_\nu, v_\nu) - \frac{(K/k)^n}{K^2-k^2} Y^m_n(u_o, v_o)\right\} \tag{11}$$

where, as before, $\underline{K}_\nu$ is the vector distance to the ν'th point in the reciprocal lattice, u_ν, v_ν are the spherical angles for the vector $\underline{K} + \underline{K}_\nu$, and v is the volume of one cell. We have subtracted off the pole at $k^2 = K^2$ for ease in computation; it will be added separately.

The wave from the p = 0 distributed source must then be subtracted off. This is zero except for m = n = 0; the second part of M is

$$\begin{aligned} M^2_{mn} &= \delta_{om}\delta_{on}\left[1 - (4\beta^3/\pi^{\frac{1}{2}}k)\int_o^\infty e^{-\beta^2r^2+ikr}\, r\, dr\right] \\ &= -\delta_{om}\delta_{on}\left[(2/\pi^{\frac{1}{2}}k)(\beta e^{k^2/4\beta^2} - k\int_o^{k/2\beta} u^2\, du)\right] \\ &= \delta_{om}\delta_{on}\,(1/\pi^{\frac{1}{2}}) \sum_{s=o}^\infty \left[(k/2\beta)^{2s-1}/s!(2s-1)\right] \end{aligned} \tag{12}$$

Finally the difference between the waves, at r = 0, due to the actual $\rho(\infty)$ and to the substituted $\rho(\beta)$ has to be added. The p'th term of this correction series is

$$(2^{n+2}\beta^n/\pi^{\frac{1}{2}}\kappa^n) i^n Y^m_n(\vartheta_p,\phi_p)\exp\left[i\underline{K}\cdot\underline{R}_p + (\kappa^2/4\beta^2)\right] S_n, \text{ where}$$

$$\begin{aligned} S_n &= \beta^{n+3}\int_{R_p}^\infty \left[J_n(kR_p)n_n(kr) - n_n(kR_p)J_n(kr)\right] e^{-\beta^2r^2} r^{n+2}\, dr \\ &= \mathrm{Im}\left\{\bar{h}_n(\gamma x_p)\int_{x_p}^\infty h_n(\gamma x) e^{-x^2} x^{n+2}\, dx\right\} \qquad (\gamma = \kappa/\beta;\ x_p = \beta R_p) \\ &= e^{-x_p^2}\mathrm{Im}\left\{h_n(\gamma x_p)\int_{x_p}^\infty e^{-2x_p(x-x_p)}\left[x^{n+2}e^{-(x-x_p)^2} h_n(\gamma x)\right] dx\right\} \end{aligned}$$

Expanding the quantity in square brackets in a Taylor's series about $x = x_p$, we obtain an asymptotic series for S_n, valid for R_p large:

$$S_n \simeq e^{-x_p^2}\sum_\sigma (2\beta R_p)^{-\sigma}\mathrm{Im}\left\{\bar{h}_n(kR_p)F^\sigma_n(\beta R_p)\right\}$$

where $F^\sigma_n(z) = \left\{d^\sigma\left[x^{n+2}e^{-(x-z)^2}h_n(\gamma z)\right]/dx^\sigma\right\}_{x=z}$

From this we finally obtain for the third part of M

$$M^3_{mn} \simeq \tfrac{1}{2} i^n (2\beta/k)^{n+1}\pi^{-\frac{1}{2}} e^{k^2/4\beta^2}\sum_{p\neq 0}(\beta R_p)^{n-2}\exp(i\underline{K}\cdot\underline{R}_p - \beta^2R_p^2)\cdot Y^m_n(\vartheta_p,\phi_p)\left[1 + \frac{(4n-2) - (\kappa/\beta)^2}{4\beta^2R_p^2} + \frac{4n^2-8n-3}{4\beta^4R_p^4} + \ldots\right] \tag{13}$$

If β is as large as 2 divided by the distance to nearest neighbor, this sum converges very rapidly, and usually only the nearest neighbor terms need to be retained if four-figure accuracy is required.

As an example, for a simple cubic lattice of spacing 2b, if we set $\beta = (\pi/8^{\frac{1}{2}}b)$ and use the dimensionless parameters

$$z = (bk/\pi);\ Z = (b\underline{K}/\pi);\ \underline{R}_{op} = (\underline{R}_p/2b) = n_x\underline{i} + n_y\underline{j} + n_z\underline{k};$$

$$\underline{Z}_\nu = (b\underline{K}_\nu/\pi) = \lambda\underline{i} + \mu\underline{j} + \nu\underline{k}\ (n_x,\ n_y,\ n_z, \lambda, \mu, \nu \text{ integers})$$

we have

$$\begin{aligned} M^o_o(Z,z) \simeq{}& \frac{1}{2\pi^2 z}\sum_\nu \frac{\exp(-2|\underline{Z}+\underline{Z}_\nu|^2 + 2z^2)}{|\underline{Z}+\underline{Z}_\nu|^2 - z^2} \\ &+ (2^{\frac{1}{2}}/\pi^{\frac{1}{2}}z)\exp(2z^2 - \tfrac{1}{2}\pi^2)\left[\cos(2\pi Z_x) + \cos(2\pi Z_y) + \cos(2\pi Z_z)\right](1 - \frac{1+4z^2}{\pi^2}) + \pi^{\frac{1}{2}}\sum_{s=o}^\infty \frac{(2z^2)^{s-\frac{1}{2}}}{s!(2s-1)} \end{aligned} \tag{14}$$

The first series requires about a hundred terms to obtain four-figure accuracy, but the task is not difficult to program for machine computation. Curves for M^o_o are given in Figure 1. The poles of the function come from the terms in the first series. If the terms for the nearest two poles be subtracted from M, the remainder can easily be interpolated to obtain intermediate values. Table I shows a few representative values. We note also that M^o_o for $\pm(\underline{Z}+n\underline{a}_x)$ equals M^o_o for $\underline{Z}$.

General Properties of the Solution - It is now possible to simplify further Equation (9). We note that only for $\ell' = \ell$, $m' = m$ is there a term in Y^o_o in the sum over n. Furthermore, $I_o(m\ell|m\ell) = (\ell+m)!/(2\ell+1)(\ell-m)!$, so that the $-i\delta_{om}\delta_{on}$ term can be combined with the first term in the curly brackets in (9). Since $h_\ell = J_\ell + in_\ell$ the J_ℓ term is cancelled out. Since, also, from the formula for the Wronskian for J_ℓ and n_ℓ, and from the definition of g^o_ℓ, we have

$$-ka(g_\ell - g^o_\ell)J_\ell(ka)n_\ell(ka) = 1 - kaJ_\ell(ka)n_\ell(ka)\left[g_\ell - \tan\beta_\ell(ka)\right] \tag{15}$$

where $\beta_\ell(z) = \tan^{-1}\left[-zn_\ell(z)/n_\ell(z)\right]$

Tables of β_ℓ have been published [5].

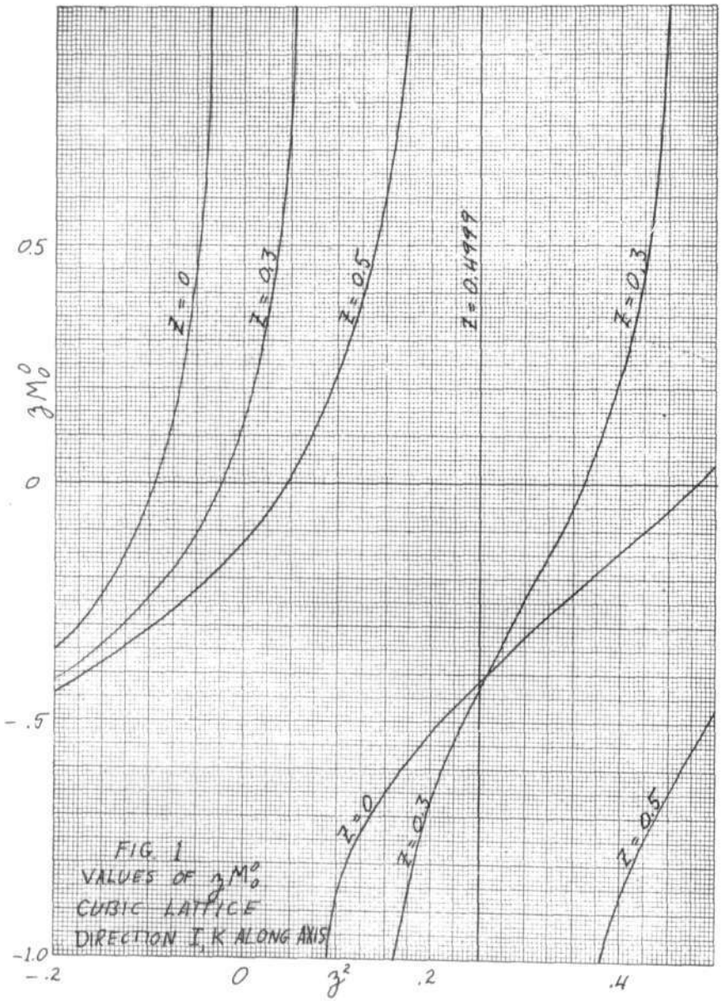

Table I Directon I, $\underline{K} = \underline{a}_x K$; Simple Cubic

Values of $zM_0^0 - \left(\frac{1}{2\pi^2}\right)\left[\frac{1}{Z^2 - z^2} + \frac{1}{(1-Z)^2 - z^2}\right]$

z^2	Z = 0	0.1	0.2	0.3	0.4	0.5
-0.4	-.7712	-.7758	-.7795	-.7823	-.7839	-.7845
-0.3	-.7110	-.7164	-.7206	-.7238	-.7258	-.7265
-0.2	-.6467	-.6530	-.6580	-.6617	-.6641	-.6649
-0.1	-.5775	-.5850	-.5909	-.5954	-.5982	-.5992
0	-.5023	-.5113	-.5185	-.5239	-.5273	-.5285
+0.1	-.4196	-.4306	-.4395	-.4462	-.4505	-.4519
0.2	-.3270	-.3409	-.3520	-.3607	-.3663	-.3682
0.3	-.2214	-.2393	-.2537	-.2651	-.2725	-.2752
0.4	-.0971	-.1211	-.1405	-.1561	-.1665	-.1702
0.5	+.0457	+.0124	-.0148	-.0372	-.0526	-.0583
	Values of $z^2 M_1^0 + \left(\frac{1}{2\pi^2}\right)\left[\frac{Z}{Z^2 - z^2} - \frac{1 - Z}{(1-Z)^2 - z^2}\right]$					
-0.4	-.03619	-.02944	-.02249	-.01524	-.00771	0
-0.3	3897	3168	2422	1644	833	0
-0.2	4222	3429	2625	1785	906	0
-0.1	4606	3737	2867	1956	995	0
0	-.05066	-.04102	-.03151	-.02156	-.01099	0
+0.1	5629	4546	3503	2407	1232	0
0.2	6333	5097	3942	2726	1401	0
0.3	7237	5797	4508	3142	1625	0
0.4	8444	6714	5263	3708	1932	0
0.5	-.10132	-.07968	-.06319	-.04517	-.02376	0
	Values of $z^3 M_2^0 - \left(\frac{1}{2\pi^2}\right)\left[\frac{z^2}{Z^2 - z^2} + \frac{(1-Z)^2}{(1-Z)^2 - z^2}\right]$					
-0.4	-.03619	-.03416	-.03226	-.03065	-.02955	-.02953
-0.3	3897	3711	3521	3349	3227	3230
-0.2	4222	4061	3869	3682	3544	3552
-0.1	4606	4479	4286	4077	3916	3930
0	-.05066	-.04991	-.04810	-.04553	-.04359	-.04378
+0.1	5629	5628	5426	5136	4892	4915
0.2	6333	6443	6228	5865	5547	5570
0.3	7237	7518	7278	6798	6365	6381
0.4	8444	8996	8704	8031	7415	7406
0.5	-.10132	-.11070	-.10712	-.09747	-.08846	-.08787

Z = (bK/π); z = (bk/π).

Lattice spacing 2b.

Finally Equation (9) becomes

$$(16)\qquad \Big[(J-1) - kaj_\ell(ka)n_\ell(ka)(g_\ell-\tan\beta_\ell)\Big]F_{m\ell} + kaj_\ell(ka)\sum_{m'\ell'} i^{\ell-\ell'}(g_{\ell'}-g^o_{\ell'})j_{\ell'}(ka) \cdot\Big[(2\ell+1)\,\frac{(\ell-m)!}{(\ell+m)!}\sum_n I_n(m\ell|m'\ell')M_n^{m'-m}\Big]F_{m'\ell'} = 0$$

where we adjust the value of k so that J-1 vanishes. The Hermitean character of the matrix components is apparent.

The factors in g are closely related to the phase angles for scattering from single spheres, for

$$(17)\qquad \frac{j_\ell(ka)(g_\ell-g^o_\ell)}{n_\ell(ka)(g_\ell-\tan\beta_\ell)} = \frac{g_\ell j_\ell(ka) + kaj'_\ell(ka)}{g_\ell n_\ell(ka) + kan'_\ell(ka)} = \tan\delta_\ell$$

In fact, when all the δ's are small except for δ_o, we can approximately reduce Equations (16) to the one for ℓ, m = 0 and, setting J-1 = 0, obtain

$$(18)\qquad k\cot\delta_o \simeq kM^o_o$$

which is an implicit equation to determine k for a given value of $\underline{K}$. To this approximation, therefore, the electronic energy k^2 (or the mean index of refraction K/k for sound waves) is determined by a term $k\cot\delta_o$, depending on the interiors of the individual spheres, and on a term M^o_o, depending on the lattice geometry.

For energies just above the potential of the interspaces (k^2 small and positive) $k\cot\delta_o$ varies slowly with K or k and M^o may be written as $(4\pi/v)(K^2-k^2)^{-1} + N^o_o$ where N^o_o is small. The form of the equation for iterative solution is

$$k^2 = K^2 - (4\pi/v)(k\cot\delta_o - N^o_o)^{-1}$$

Near a resonance level of the atom $k\cot\delta_o$ goes to infinity: In this case the form (18) is more appropriate for iterative solution. Near the edge of a Brillouin zone M^o_o becomes very large, so that this is the dominant term. Having curves for $k\cot\delta_o$ and kM^o_o as functions of k for a given $\underline{K}$, graphical solutions can be obtained fairly easily, as long as only δ_o is large enough to be worth including.

When δ_ℓ for $\ell>0$ is small but not negligible, we can solve Equation (18) first to obtain a first approximation for k, substitute this in the following equation for the coefficients F,

$$(19)\qquad F_{m\ell} \simeq i^\ell(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}\,\frac{g_o j_o(ka)+kaj'_o(ka)}{g_\ell n_\ell(ka)+kan'_\ell(ka)}\,\Big[(\cot\delta_o-M^o_o)(-1)^\ell \cdot \bar{Y}^m_\ell(u_o,v_o) + M^{-m}_\ell\Big]F_{oo}$$

where, as mentioned before, u_o, v_o are the spherical angles for the vector $\underline{K}$. A next approximation for k^2 can then be obtained by substituting back in the equation for F_{oo}.

When δ_ℓ or δ_o are not so small that their squares can be neglected, then the determinent of the coefficients of Equation (16) must be set equal to zero and solved in its entirety. Since, in most cases of interest, δ_ℓ can be neglected for $\ell>2$, it is seldom necessary to solve a determinant of larger than third order. In practice, the approximations of Equations (18) and (19) are quite good for the elements of the first row of the periodic table [9], and a two-by-two determinant is sufficient for sodium to potassium.

It is sometimes convenient to expand the solutions in the field-free inter-space in terms of plane waves. This can now be done, after the F's and k have been computed for a given K, by using Equation (5) and the plane wave expansion for 0 given in Equation (4). The second term in the integrand of (5) may easily be integrated, using (2) and a relation [4] between the Y's and j's. The first term may also be simplified, using the relation

$$\int Y^m_\ell(\vartheta_o,\varphi_o)\,\cos u_\nu\cos\vartheta_o + \sin u_\nu\sin\vartheta_o\cos(\varphi_o-v_\nu)\,e^{-(\underline{K}+\underline{K}_\nu)\cdot\underline{a}_o}\,d\Omega_o = 4\pi i(-1)^\ell j_\ell(|K+K_\nu|a)\,Y^m(u_\nu,v_\nu)$$

Combining the two, we see that, in the interspaces

$$(20)\qquad \Psi = \frac{4\pi a}{v}\sum_\nu \frac{\exp\big[i(\underline{K}+\underline{K}_\nu)\cdot\underline{r}\big]}{|\underline{K}+\underline{K}_\nu|^2 - k^2}\Big\{\sum_{m\ell}(-1)^\ell\Big[g_\ell - g^o_\ell(|\underline{K}+\underline{K}|\,a)\Big]\cdot j_\ell(|\underline{K}+\underline{K}|\,a)Y^m_\ell(u_\nu,v_\nu)F_{m\ell}\Big\}$$

This equation can, of course, also be used as a basis [3] for a set of equations determining the F's or the coefficients B_ν of the plane waves of Equation (3). But the convergence of this series is much less rapid than the series in the F's, so it is much easier to use Equation (16) or (9) to determine k and the F's and then compute series (20) if needed, rather than to use Equation (20) to determine k and the F's.

Tables of the M's are now being computed by the Project.

Philip M. Morse

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[1] J. C. Slater, Phys. Rev. 51, 846 (1937).

[2] J. Korringa, Physica, 13, 392 (1947).

[3] W. Kohn and N. Rostoker, Phys. Rev. 94, 1111 (1954).

[4] See Morse and Feshbach, "Methods of Theoretical Physics" McGraw-Hill Book Company, page 1467.

[5] See, for example, "Tables of Amplitudes and Phase Angles for Scattering from Cylinders and Spheres" N.D.R.C.-M.I.T. Report No. 62.1R, 6.1-sr1046-2032, reprinted 1950 by O.N.R.

[6] L. L. Foldy, Phys. Rev. 67, 107 (1945).

[7] We might call these functions Ewald or Madelung functions.

[8] P. P. Ewald, Phys. Rev. 67, 107 (1945).

[9] P. M. Morse, Rev. Mod. Phys. 4, 580 (1932).

ENERGY BANDS IN GRAPHITE

In an earlier report [1] an unsatisfactory tight-binding calculation of a two-dimensional graphite model was described wherein the overlap matrices were not positive definite for certain values of K, the reciprocal lattice vector. A tentative conclusion was drawn that the cause of the difficulty was a result of only including overlap integrals up to third nearest-neighbors. Since then, considerable time has been spent writing and testing a more elaborate matrix generation computer program which allows the inclusion of up to ninth nearest-neighbor integrals in both the Hamiltonian and overlap matrices. On the basis of the new matrix generation program, the hypothesis of insufficient overlap integrals was found to be the correct interpretation of the previous unsatisfactory calculation. Further investigation is being made to determine the number of overlap integrals which are significant.

An additional test has also been made to investigate the importance of the heretofore neglected three-center integrals of the Hamiltonian matrices. Two sets of results, consisting of the energy eigenvalues at several representative k values, were obtained: The first set was computed with all three-center integrals neglected; the second set was computed with estimates made of the three-center integrals. These two sets of results differed markedly, and therefore it appears that at least the most important three-center integrals must be accurately included in this type of calculation.

At the present time these required three-center integrals are being computed using the multi-center integral techniques described briefly in the previous progress report; namely, that of expanding all wave functions and potentials about a single center and performing the resultant one-center integrals numerically. Final tests of the computer programs necessary for this procedure are currently being made. Preliminary results indicate excellent agreement with the previous two-center integral values (obtained by the different technique of evaluating analytic functions). Thus, the extra labor of obtaining the three-center integrals has some

compensations in that it forms an independent cross-check of a large part of the numerical work.

Fernando J. Corbato

Reference:

[1] F. J. Corbató, Quarterly Progress Report, Solid-State and Molecular Theory Group, M.I.T., October 15, 1954, p. 5.

VARIATIONAL DETERMINATION OF ATOMIC WAVE FUNCTIONS

The Whirlwind program for carrying out the variational calculations for the Morse-Young three parameter wave functions has been nearly completed. A thorough recalculation of the original energy tables as well as the calculation of several new states such as $(1s^2 2s^2 2p^5)^2P$ will be started shortly.

The gradient method mentioned in Progress Report No. 15 works very well as long as the parameters are of approximately equal strength. This condition is not satisfied for states with many 2p electrons and we have a situation like the one indicated schematically in Figure 1.

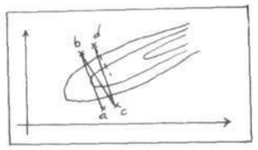

Figure 1
Energy Contour Diagram

a, b, and c represent the successive points determined by the machine in trying to reach the extremum. The narrow hill makes the path to the top extremely indirect and lengthy.

To remedy this, the program has been modified in a manner illustrated in Figure 2. An initial guess (A) of the best parameter values is made and the gradient is calculated. We then proceed along the gradient line until we reach an extremum (A'). At (A') we again calculate the gradient and move in its direction to (B). Starting at (B), we then move along a line parallel to $\overline{AA'}$ until extremum (B') is found. Finally, we move along $\overline{A'B'}$ until we reach (E') which is taken as the approximate minimum point. This process may be iterated if necessary. The various minima are found by linear interpolation of derivatives obtained by taking first differences.

When applied to states with five or six 2p electrons such as $(1s^2 2s^2 2p^5)^1s$, the above procedure gives satisfactory results.

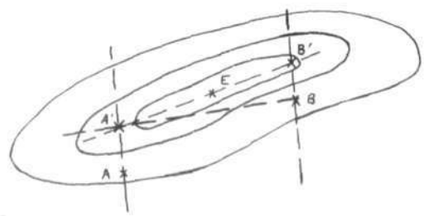

Figure 2

An effort is now being made to improve the wave functions by adding extra parameters. The most attention is being given to the 1s and 2p functions. The forms now being investigated are

$$1s \qquad \mu_1 = N_1(e^{-\mu ar} + Be^{-\mu \delta ar})$$

$$2p \qquad \mu_3 = N_3(r^2 e^{-\mu \delta' cr} + B' r^2 e^{-\mu \delta' cr}) P_1^0(\cos\varphi)$$

The values of B and δ have been calculated for the helium isoelectronic sequence and it is hoped that these will hold for any configuration containing two 1s orbitals.

Arnold Tubis

SCATTERING OF SLOW ELECTRONS FROM ATOMIC OXYGEN

The physical aspects of this problem have been discussed in the various thesis reports. Roughly they can be summed up as an extension of the Hartree-Fock method to a continuous state problem. Mathematically the problem is to solve a set of second-order integro-differential equations. The equations are of the form

$$\frac{d^2u}{dx^2} + f(x)u(x) + g(x, C^{(k)}, \int_0^x p(x')u(x')dx') = 0$$

$p(x')$ is a known function. The constants $C^{(k)}$ are integrals from 0 to ∞ over the unknown function:

$$\int_0^\infty x'^k p(x')u(x')dx'$$

To solve these equations, the procedure is to take a guess at $C^{(k)}$ and to solve the equations using these guessed values for the $C^{(k)}$. This gives the function u from which one can evaluate the integral $C^{(k)}$ and use this as a next guess; i.e., one uses an iterative procedure which presumably will converge.

The equations solved thus far were s-wave equations for the total S = 1/2 case (spin of incoming electron opposite to the S = 1 spin of atom). In this case the angular integrations make the integral part of the equation vanish and the equation is just an ordinary differential equation.

$$\frac{d^2u}{dx^2} + u\left\{(a_o k)^2 - 8G_1(x)\right\} = 0$$

G(x) is a known, tabulated function which depends on the numerical Hartree-Fock wave function for the oxygen atom; $(a_o k)^2$ is proportional to the energy. Actually we are interested in the phase shifts and these have been computed by Whirlwind to be, for various values of the energy:

(in radians)	$(a_o k)$	Energy (in e.v.)
-3.11	.1	.136
-3.09	.2	.545
-3.07	.3	1.22
-3.07	.4	2.18
-3.07	.5	3.40
-3.08	.6	4.90

Aaron Temkin

NEUTRON-DEUTRON SCATTERING

It has been found that the n-d scattering lengths are much more sensitive to the accuracy of the assumed deuteron wave function than was previously believed to be the case. From Equations (16) and (19) of the previous report [1], we can form the integral expression

$$(1)\qquad \int \frac{d\tau}{r_1 r_2} \Big\{ (\omega_2 - \bar{\omega}_2) T (\omega_1 - \bar{\omega}_1) - (\omega_1 - \bar{\omega}_1) T (\omega_2 - \bar{\omega}_2) + r_{12} \Big[(\omega_2 - \bar{\omega}_2)(\Omega_{13} \frac{\omega_1}{r_{12}} - \Omega_{13} \frac{\bar{\omega}}{r_{12}}) - (\omega_1 - \bar{\omega}_1)(\Omega_{23} \frac{\omega_2}{r_{12}} - \Omega_{13} \frac{\bar{\omega}_2}{r_{12}}) \Big] \Big\}$$

where ω_1, ω_2, $\bar{\omega}_1$, $\bar{\omega}_2$ involve the deuteron function and are defined in ([1], 15, 18). On applying Green's theorem to the second derivatives contained in T, we can write (1) in the form

$$(2)\qquad L_1 + L_2 = \int \frac{d\tau}{r_{12}} \Big[\omega_1 \Omega_{13} \frac{\bar{\omega}_2}{r_{12}} + \bar{\omega}_1 \Omega_{23} \frac{\omega_2}{r_{12}} - \omega_2 \Omega_{13} \frac{\bar{\omega}_1}{r_{12}} - \bar{\omega}_2 \Omega_{23} \frac{\omega_1}{r_{12}} \Big]$$

where L_1 is the surface integral defined in ([1] 27b) and L_2 is another surface integral of the same type. Equation (2) is satisfied identically if in ω_1, ω_2, $\bar{\omega}_1$, $\bar{\omega}_2$ we use the exact deuteron function; with any approximate deuteron function, the left and right-hand sides of the equation will differ. This difference leads us to the formulation of a variational principle slightly different from the one developed in ([1] 29), which we shall denote as A. The alternate form, which we denote as B, is obtained by adding (2) to equation ([1]26) and then proceeding exactly as in the original derivation. Since the terms added do not involve the trial function ψ, the stationarity of the resulting equation with respect to variations in ψ is unaffected. Variational principles A and B are, of course, identical in the limit of exact deuteron function.

The deuteron wave function which has been used thus far in the calculations is of the form

$$(3)\qquad F(r) = e^{-\alpha r^2} + c e^{-\beta r^2}$$

where the constants α, β, c are determined by an independent variational calculation to minimize the energy of the deuteron ground state. (A Gaussian form for the deuteron function is required in order to perform the integrations.) The form (3) gives a binding energy which differs from the experimental value by about .2 MEV, which is quite small in comparison with the kinetic and potential energies involved. It was therefore believed that (3) would be an adequate function to use in the calculations.

However, in Equation (2), which is not stationary, the use of (3) as a deuteron function leads to a difference of about 20 per cent between the left and right-hand sides. The reason for this large difference is mainly that L_2 turns out to involve the correlation between the deuteron function at small and large values of the argument. At large distances the wave function (3) is the poorest, a fact which does not greatly affect the binding energy.

As a result of this 20 per cent difference in Equation (2), we find that the variational principles A and B give results which also differ substantially. Various plausibility arguments lead us to believe that A is more accurate, but are not completely convincing. In an effort to resolve the uncertainty, it has been decided to redo the calculations using a more accurate deuteron function. Christian and Gammel [2] give a deuteron function of the form

$$(4)\qquad F(r) = e^{-\alpha r^2} + c_1 e^{-\beta r^2} + c_2 e^{-\gamma r^2}$$

which approximates the exact solution within three per cent and leads to a difference of only five per cent between the two sides of Equation (2). (4) should therefore be completely adequate for our purposes.

The use of (4) as a deuteron wave function introduces no intrinsic complications in the computation. It does, however, increase the number of terms to be evaluated and will require additional programming and machine time. However, the relative ease with which the stationary point was found using wave function (3) indicates that the additional machine time should not be excessive. The reprogramming is now in progress.

Leo Sartori

References:

[1] Machine Methods of Computation, Quarterly Progress Report No. 15, p. 23, March (1955).

[2] R. S. Christian and J. L. Gammel, Phys. Rev. 91, 100 (1953).

EIGENVALUES FOR A SPHEROIDAL WELL

In order to compute the matrix elements described in the previous quarterly report, it is necessary to compute the logarithmic derivatives of the two "radial" spheroidal functions $je_{m\ell}(h,a)$ $he_{m\ell}(ig,a)$. As before, we have

$$h^2 + g^2 = H^2;\ H^2 = d^2 V_0$$

where d is the focal length of the (prolate) spheroid and v_0 is the well depth while a is the value of the radial parameter at the boundary of the well. The $je_{m\ell}$ function is finite at $a = +1$ and behaves asymptotically as a spherical bessel function. The $he_{m\ell}(ig,a)$ blows up at $a = 1$ and has the asymptotic behaviour of a spherical Hankel function of the first kind and of argument iga.

Now it can be shown that the $je_{m\ell}$ function may be expanded in a series of spherical Bessel functions as [1]

$$(1)\qquad je_{m\ell}(h,a) = \Big(\frac{a^2-1}{z^2}\Big)^{m/2} \sum_{n=0}^{\infty} a_{2n+p}(h|m\ell)\, j_{2n+m+p}(ha)$$

p = 0 for (ℓ-m) even

p = 1 for (ℓ-m) odd

The a 's are computed on a demand basis by a subroutine which was developed by Mr. F. J. Corbató and Dr. J. D. C. Little. Computation of the spherical Bessel functions was carried out by the method described in part II of this report.

By examining the differential equation for the "radial" function [2], one sees that the prolate spheroidal function $he_{m\ell}(ig,a)$ is identical to the oblate spheroidal function $he_{m\ell}(g,ia)$. Although this function may also be expanded in a series similar to that in Equation (1) (with the j_n's replaced by h_n's of the first kind), it turns out that the series converge very slowly or not at all. Consequently, it was necessary to find a different method for computing this function.

A suggestion as to a possible method may be obtained from the asymptotic behavior of the $he_{m\ell}$ function. Suppose we choose two arbitrary numbers $\alpha_{m\ell}$, $\beta_{m\ell}$ and a value z_0 such that $z_0 >> a$. Now let $\alpha_{m\ell}$ be the value and $\beta_{m\ell}$ the derivative of a solution of the radial spheroidal equation at z_0. Then we can write

$$\alpha_{m\ell}(z_0) = a_1 he_{m\ell}(q_1, iz_0) + a_2 je_{m\ell}(q_1, iz_0)$$

$$\beta_{m\ell}(z_0) = (\partial/\partial z_0)\big[a_1 he_{m\ell}(q_1, iz_0) + a_2 je_{m\ell}(q_1, iz_0)\big]$$

Now $he_{m\ell}(g,iz)$ not only behaves as a decreasing exponential for sufficiently large values of z, but it must be a monatonic decreasing function throughout its range. On the other hand, $je_{m\ell}(g,iz)$ must increase monotonically throughout its range, going asymptotically as e^{gz}/gz. Thus, by choosing z_0 sufficiently large and integrating the differential equation for the radial equation inward from z_0 to a, taking $\alpha_{m\ell}(z_0)$, $\beta_{m\ell}(z_0)$ as initial conditions, we can get to a high degree of accuracy that

$$\alpha_{m\ell}(a) \approx a_1 he_{m\ell}(q_1, ia)$$

$$\beta_{m\ell}(a) \approx a_1 \Big[\frac{\partial}{\partial z} he_{m\ell}(q_1, iz)\Big]_{z=a}.$$

Moreover, since it is only the logarithmic derivative of $he_{m\ell}$ that is of interest, the value of the constant a_1 is of no concern.

This scheme is now in use for computing the desired function. The constants $\alpha_{m\ell}(z_0)$, $\beta_{m\ell}(z_0)$ are so chosen that their ratio $\beta_{m\ell}(z_0)/\alpha_{m\ell}(z_0) = -g$ which guarantees that a^2/a_1 will be small to begin with. By using a second order integration process with an increment Δz determined so that $g\Delta z = .025$ and choosing z_0 so that $g(z_0 - a) \approx 6$, it was found that

$$\Big[\frac{d}{dz} \ln he_{m\ell}(q_1, iz)\Big]_{z=a}$$

could be obtained with an error of less than about three per cent in a time of about fifteen seconds.

II. Computation of Spherical Bessel Functions[1] [2]

The spherical Bessel, Hankel, and Neumann functions of order n all obey the equation

$$(1)\qquad \Big\{ \frac{1}{x^2} \frac{d}{dx} x^2 \frac{d}{dx} + \Big[1 - \frac{n(n+1)}{x^2}\Big] \Big\} y_n = 0$$

---

[1] Equations (1)-(4) may be found in [3, pp. 1573-4].

or, equivalently, the difference equation

(2) $\psi_{n-1}(x) = \frac{2n+1}{x}\psi_n(x) - \psi_{n+1}(x)$

In particular we shall take the two independent solutions of (1) to be the spherical Bessel function, $j_n(x)$ and the spherical Neumann function $n_n(x)$. These functions may be conveniently defined in terms of initial conditions on the difference Equation (2). Thus,

(3) $j_{-1}(x) = \frac{\cos x}{x}$ $\qquad n_{-1}(x) = -\frac{\sin x}{x}$

$j_0(x) = \frac{\sin x}{x}$ $\qquad n_0(x) = -\frac{\cos x}{x}$

In addition to Equations (1) and (2), we shall also make use of the relation

(4) $\int x^{n+2}\psi_n(x)\,dx = x^{n+2}\psi_{n+1}(x)$.

If we set $y_n(x) = \frac{1}{x}z_n(x)$, Equation (1) becomes

$\left\{\frac{d^2}{dx^2} + \left[1 - \frac{n(n+1)}{x^2}\right]\right\} Z_n(x) = 0$.

Thus, we see that the n-x plane may be divided into two regions according to

(I) $x^2 < n(n+1)$; (II) $x^2 > n(n+1)$

and the behaviour of the solutions will be essentially different in each region. In fact, it is not difficult to show that in region (I) $\frac{1}{x}j_n(x)$ is a monotonic increasing (positive) function of x and $1/x\, n_n(x)$ is a monotonic decreasing (in magnitude) negative function of x. On the other hand, both functions are oscillatory in region (II).

In most of what follows we shall be concerned with the behaviour of the two functions in region (I). The discussion will involve two numbers N,t which are defined by:

(d_1) For fixed x, N is the least integer such that $N(N+1) \geq x^2$.

(d_2) For fixed n, t is any positive number such that $t^2 < n(n+1)$.

Using the above definitions together with Equation (4) and the known behaviour of $1/x\, j_n(x)$ in region (I), we see that

$\int_0^t x^{n+2} j_n(x)\,dx = t^{n+2} j_{n+1}(t) < \frac{1}{t} j_n(t) \int_0^t x^{n+1}\,dx$

or

$j_n(t) > \frac{n+1}{t} j_{n+1}(t)$

which leads to the relation

(5a) $\frac{j_n(x)}{j_N(x)} < x^{n-N}\frac{(N+3)!}{(n+3)!}$, $n > N$

A trivial modification of the above argument leads to the conclusion that

(5b) $\frac{n_N(x)}{n_n(x)} < x^{n-N}\frac{(N+3)!}{(N+3)!}$

In order to make use of these inequalities, we define for $n \gg N$

$\bar{j}_{n+1}(x) = \alpha[j_{n+1}(x) + \beta n_{n+1}(x)]$

$\bar{j}_n(x) = \alpha[j_n(x) + \beta n_n(x)]$

where $\bar{j}_{n+1}(x)$ and $\bar{j}_n(x)$ are any two arbitrarily chosen numbers. Repeated application of Equation (2) then gives

$\bar{j}_N(x) = \alpha j_N(x)\left[1 + \beta\frac{n_N(x)}{j_N(x)}\right] = \alpha j_N(x)(1+\delta)$.

Now make the special choice $\bar{j}_{n+1}(x) = 0$. Then, by making use of the inequalities (5), we find that

(6) $\delta < x^{2(n-N+2)}\left[\frac{(N+3)!}{(n+4)!}\right]^2$

Table I gives a few values of n vs. N with n so chosen that $\delta < 10^{-10}$.

Table I

N = 1	5	10	15	20	25
n = 7	17	25	35	42	50

The inequality (6) suggests a method for computing sets of functions $j_k(x)$ (x fixed, $n_1 \leq k \leq n_2$) which appears to be ideally suited for a high-speed digital computer. We first put the larger of the two integers (n_2, N) in place of N in (6) and choose n to make δ less than some specified amount. Next take $j_n(x)$ to be any convenient number and $j_{n+1}(x) = 0$. The recursion relation (2) is then used to generate the set of numbers $j_k(x) \ni j_{n_1}(x)$, which is left stored in the machine and also the numbers $j_0(x)$, $j_{-1}(x)$. Use of either of these last two quantities together with the appropriate one of the Equations (3) allows us to compute the normalization constant, $1/\alpha$, and, consequently, the $j_k(x)$.

In the event that x (and, in consequence, N) is very large, it will be necessary to generate many values which lie in region II in order to obtain j_0. We have seen that use of Equation (2) in region I leads to "damping" of the round-off error introduced at each step. The same effect does not occur in region II. Instead, we should expect the successive contributions of round-off error to add in random fashion with a resulting loss of accuracy in the computation of the normalization constant α. My experience has been that this effect is negligible for x as high as 25 (computations carried out on Whirlwind using 24, 6 arithmetic).

In carrying out the computations, a slight modification of the above method was used. It was found that cases occur where $j_n(x)$ cannot be chosen sufficiently small so that $j_N(x)$ does not exceed the storage capacity of the machine. This difficulty was avoided (and the computing time decreased) by using Equation (2) in the form

(2a) $r_{n-1} = \frac{x}{2n+1-x r_n}$, $r_n = \psi_{n+1}(x)/\psi_n(x)$,

and computing with the ratios throughout region I.

Jack L. Uretsky

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A SELF-CONSISTEN DETERMINATION OF THE NUCLEAR RADIUS

A Hartree-Foch type of self-consistent field problem has been set up and solved for a standard heavy nucleus of 22 = 2N = A = 184.

The purpose of the calculation is to determine the relation between nuclear matter distribution and the resulting collective nuclear potential. As a first trial, internuclear forces were considered to be Wigner plus Majorana, the radial dependence of the force being Gaussian:

$$V = 43e^{-.5r^2}[1+xP(rr')]$$

P(rr') is the Majorana exchange operator, and x is the ratio of Majorana to Wigner force. The following is an outline of the method of solution:

(a) A square well of radius 8.2 fermis ($= 1.4 \times 184^{1/3}$) and depth 32 Mev is filled with 184 non-interacting particles; 46 neutrons with spin up, 46 with spin down and 46 protons with spin up, 46 with spin down.

(b) The wave functions for this well are used to calculate the density distribution of the particles.

(c) The collective potential generated by these is calculated using the assumed internucleon potential.

(d) A new set of wave functions is derived from the new effective potential, and from these wave functions a new density distribution is obtained.

(e) Steps (c) and (d) are repeated until the potential is the same for two iterates.

It was found that the process converged after a single iteration when x was slightly greater than 4. The significant result of the calculation is that for the self-consistent solutions the mean square radius of the potential is 41.4 fermis, and that of the matter distribution 38.4 fermis, so that the root mean square radius of the potential is only four per cent larger than the matter distribution which produced it. Further calculations with Yukawa forces and other exchange admixtures are now in progress.

Manuel Rotenberg

DYNAMIC BEHAVIOR OF SHEAR WALL TESTING MACHINE

The shear wall testing machine is composed of two trusses and connecting bracing. The concrete wall to be tested is placed on the frame between the two trusses and the dynamic load is applied by a hydraulic system.

For the elastic-plastic stress analysis the testing machine and the concrete test wall are represented by a twenty mass system connected by elastic-plastic springs. The masses representing the testing machine are located at the truss joints and are composed of 1/2 of the mass of each member coming into the joint. Since the truss joints will all be assumed pin connected (no moment resistance), the resistance of each member will be composed of just the axial force.

The behavior of each mass point can be represented by an equation of the form:

$$M_i \ddot{X}_i(t_n) = P_{Xi}(t_n) - \sum R_{Xi}(t_n)$$

where:

M_i = mass at joint i
$X_i(t_n)$ = displacement of mass i in the X direction at time t_n
$\sum R_{Xi}(t_n)$ = sum of the resistances at joint i in the X direction at time t_n

The twenty simultaneous equations will be numerically integrated by use of terms through the first backward difference of the difference equation:

$$X_i(t_{n+1}) = 2X_i(t_n) - X_i(t_{n-1}) + (\Delta t)^2\left[1 + 0\nabla + \tfrac{1}{12}\nabla^2 + \tfrac{1}{12}\nabla^3 + \ldots\right]\ddot{X}_i(t_n)$$

The results will be checked by use of the fourth order Kutta-Gill integration procedure from the Whirlwind subroutine library.

We are planning on running solutions for a large number of loading conditions as well as several conditions of support.

Charles W. Johnson

ANALYSIS OF A TWO-STORY STEEL FRAME BUILDING UNDER DYNAMIC LOADING

With the program discussed in the last quarterly report, we have carried out a large number of calculations for a wide range of resistance functions and loading conditions. We also decided to make some small modifications in the original program so that we could investigate another group of resistance functions. This new program has now been written, and we have run solutions for most of the resistances.

Charles W. Johnson

RESPONSE OF A FIVE-STORY FRAME BUILDING TO DYNAMIC LOADING

During the last quarterly period, we have run a number of analyses of the building frame using loads of verying intensity and duration. We have also checked one Whirlwind solution with a desk calculator computation. The magnitudes of the amplitude of these two solutions agree very closely and there is only a slight phase shift between the peaks.

We hope to finish the analysis of this particular building in the next two weeks. We will then use the same program to analysis a similar building.

Charles W. Johnson

2.3 Final Reports

MACHINE SOLUTION OF THE DIFFUSION EQUATION

A description of this problem is given in the preceeding reports [1] along with a general form for the analytic solution and an outline of a numerical approach to the solution [2] using a difference equation formulation for variable spacing. Since then, a number of runs using an example have been made with the I.B.M. Card Programmed Calculator and some definite conclusions have been made. Also, the question of the stability conditions (the behavior of an error propogation) has been investigated and will be reported on here.

The general problem is

(1) $$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left[K(x)\frac{\partial U}{\partial x}\right], \quad K(x) > 0$$

in $0 \leq x \leq L$, and initial and boundary conditions

$$-K(x)\frac{\partial U}{\partial x}\Big|_{x=0} = Q, \quad 0 < t$$
$$\frac{\partial U}{\partial x}\Big|_{x=L} = 0, \quad 0 < t$$
$$U(x,0) = 0, \quad 0 < x < L.$$

The difference equation formulation [3] used is

(2) $$U_{n,m+1} = A_{n,j}U_{n-1,m} + B_{n,j}U_{n,m} + C_{n,j}U_{n+1,m}$$

where
$$A_{n,j} = \frac{jk(2K_n - h_n K'_n)}{h_{n-1}(h_n + h_{n-1})}, \quad B_{n,j} = 1 - \frac{jk(2K_n - (h_n - h_{n-1})K'_n)}{h_n h_{n-1}}$$
$$C_{n,j} = \frac{jk(2K_n + h_{n-1}K'_n)}{h_n(h_n + h_{n-1})}$$

and
$$U_{n,m} \equiv U(x_n, t_m), \qquad x_n = \sum_{i=1}^{n} h_i, \quad t_m = mk$$
$$K_n = K(x_n), \qquad n = 0,1,2,\ldots,N; \quad m = 0,j,2j,3j,\cdots$$

The boundary conditions are now

(3) $$U_{-1,m} = U_{1,m} + hQ/K_0$$
$$U_{N-1,m} = U_{N+1,m}$$

Since the solution of (2), with variable coefficients, is practically impossible, the case for constant coefficients will be discussed. It is easily seen that a sufficient condition for (2) together with (3) to be stable is that its domination coefficient formulation also be stable [4]. Thus, stability conditions of the problem

(4) $$U_{n,m+1} = AU_{n-1,m} + BU_{n,m} + CU_{n+1,m}$$
$$U_{-1,m} = U_{1,m}, \qquad U_{N-1,m} = U_{N+1,m}$$

will be discussed. The property A + B + C = 1 is to still hold.

The term stability as is used here refers to the manner in which an error propagates. When an error of the type studied here occurs, it would be due to round-off or gross mistakes and consequently can be represented as $U_{n,m} = C\delta_{n,m}$, [5], the kronecker delta. This would comprise the initial condition of (4). The error must satisfy (4) together with the boundary conditions which would be homogeneous as far as the error is concerned. Further, the error itself will have a product form of solution. Thus, suppose $U_{n,m} = N_n M_m$, so,

(5) $$\frac{M_{m+1}}{M_m} = \frac{CN_{n+1} + BN_n + AN_{n-1}}{N_n} = \Lambda$$

The solution of the first equality is $M_m = \Lambda^m$. It is immediately apparent that if

$$|\Lambda| > 1, \quad |\Lambda| = 1, \quad |\Lambda| < 1$$

the error will grow exponentially, linearly, or decay exponentially, respectively. The second equality in (5) is

$$N_{n+1} + \frac{B}{C} N_n + \frac{A}{C} N_{n-1} - \frac{\Lambda}{C} N_n = 0$$

provided $C \neq 0$. Setting

$$\frac{\Lambda}{C} = \frac{B}{C} + 2\sqrt{\frac{A}{C}} \cos\alpha \tag{6}$$

The solution [5] has the form

$$N_n = \left(\frac{A}{C}\right)^{\frac{n}{2}} \left[a \cos\alpha n + b \sin\alpha n\right]$$

where a and b are constants. Complex values of α are not excluded. Applying the boundary conditions and considerable algebraic manipulation, α may be determined from the relation

$$(\sin\alpha N)\left[\cos 2\alpha - \tfrac{1}{2}\left(d^2 + \tfrac{1}{d^2}\right)\right] = 0 \tag{7}$$

where $d^2 = \frac{A}{C}$. Thus, $\alpha = \frac{\pi r}{N} = \alpha_r$ for r = 1, 2, 3,..., N-1 (the value r = 0 yields a zero eigenfunction). Also, the case

$$\cos 2\alpha_N = \tfrac{1}{2}\left(d^2 + \tfrac{1}{d^2}\right)$$

is another perfectly good zero of (7) and when substituted into (6) gives $\Lambda = 1$. A total of N eigenvalues are found as would be expected. So, the condition $|\Lambda| \leq 1$ can be stated

$$|B + 2\sqrt{AC}\cos\alpha_r| \leq 1 \quad \text{for all } r. \tag{8}$$

It is indeed sufficient for purposes of stability to require that all coefficients be positive or zero and thus less than unity:

$$|B + 2\sqrt{AC}\cos\alpha_r| \leq |B + 2\sqrt{AC}| < |B + A + C| = 1.$$

It will be noticed that for some values of B<0 and A ≠ C (8) will still hold for all α_r. Likewise, some negative values of either A or C are not excluded.

A second and even more difficult question to answer is that of convergence. Under what conditions does the difference equation solution converge to the solution of the differential equation? A complete answer to this question is unknown.

A Numerical Example

A numerical example has been worked out and the results will be described here. Let K = x + b, L = 895, b = 2, Q = 1 in problem (1). Also, let us adopt the rule that all coefficients in (2) are positive or zero. It will be seen that spacing in the x direction may be taken according to

$$x_n = 2^n - 1, \quad x_{-1} = -1$$

will satisfy the above stability conditions. Table I gives the manner in which the spacing was chosen and the resulting coefficients. Constant spacing was resorted to for n>7. As a direct result of this, the j values had to be decreased in order to maintain positiveness of the coefficients.

The next step involves combining the difference equations ("telescoping") in such a way as to obtain a constant j value for the whole interval (0, 895). The method for doing this is described in [2]. The resulting difference equations are of the form

$$U_{n,m+64} = \sum_i a_{n,i} U_{i,m} + \bar{a}_n, \quad n = 0, 1, 2, \cdots, N. \tag{9}$$

These new coefficients are listed in [3] for n≤6. It will be noted that (9) reduces to (2) for n = 7, 8 and 9. Also, $\bar{a}_n = 0$ for n≥7. $U_{10,m+64}$, $U_{11,m+64}$,..., $U_{13,m+64}$ are all readily calculated from Table I. Thus:

$$\begin{aligned} U_{10,m+64} &= A_{10,32} U_{9,m+32} + B_{10,32} U_{10,m+32} + C_{10,32} U_{11,m+32} \\ &= (A_{10,32} A_{9,32} &&) U_{8,m} \\ &+ (A_{10,32} B_{9,32} + B_{10,32} A_{10,32} &&) U_{9,m} \\ &+ (A_{10,32} C_{9,32} + B_{10,32} B_{10,32} + C_{10,32} A_{11,32} &&) U_{10,m} \\ &\quad + (B_{10,32} C_{10,32} + C_{10,32} B_{11,32} &&) U_{11,m} \\ &\quad + (C_{10,32} C_{11,32} &&) U_{12,m} \end{aligned}$$

and similarly for $U_{11,m+64}$, $U_{12,m+64}$,..., $U_{14,m+64}$. Of course the boundary conditions (3) are used when appropriate.

If one were to program this problem at this stage and run it off on a high-speed computer, then compare the steady state with the analytic steady state, one would find that the formulation as it has been set up here so far does not converge to the analytic steady state solution [3]! It is believed that the reason for this is that the left-hand boundary condition (3) which "feeds in the heat" is a very bad approximation to the actual boundary temperature since the singularity at x = - b = - 2 is so near. A way of getting around this difficulty [2] is to require the condition

$$\int_0^L U(x,t)\,dx = QT. \tag{10}$$

That is to say, by integrating over the interval (0,L) numerically, then adjusting the boundary value so that (10) is approximately satisfied, this difference equation formulation may be made to converge to the proper steady state solution. An alternative method is to adjust the Q so as to obtain the proper head in-flow [3]. In a very similar problem [3] variable spacing across the entire interval (0,L) was used and again there was difficulty with convergence even though (10) was enforced. It is believed that this was due to the fact that in spite of the higher derivatives present in the truncation error associated with (2) being very small, the exponentially increasing h_i tended to make them significant.

Table II presents some of the intermediate and final results of the example problem used here. The test for the dominance of the steady state is very simple. It will be remembered that in the analytic solution there is a Qt/L term. If one applies a forward difference operator with respect to t (with spacing constant Jk) to the steady state analytic solution (11), there remains the term

$$\frac{Q}{L}\Delta t.$$

Or

$$\frac{Q}{L}\Delta(mJk) = \frac{QJk}{L} = \frac{16}{895} = .0178771.$$

If one applies this operator to the CPC values of $U_{n,m}$, one should expect to get very nearly this numerical value over the entire interval $(0,L)^{n,m}$. This test was used to determine the steady state dominance in this example. At m = 4480

$$\Delta U_{0,4480} = .01902, \quad \Delta U_{N,4480} = .01741$$

whereas

$$\Delta U_{0,8000} = .01790, \quad \Delta U_{N,8000} = .01786$$

and

$$\Delta U_{0,9152} = .\emptyset 1788, \quad \Delta U_{N,9152} = .01787.$$

The analytic steady state values [3] were calculated from

$$U = \left(\frac{L+b}{L}\right)^2 \ell_n \frac{L+b}{b} - \frac{1}{2}\left(\frac{3L+2b}{L}\right) + Q\left[\frac{x}{L} - \frac{L+b}{L}\ell_n\frac{x+b}{b}\right] + \frac{Qt}{L}. \tag{11}$$

The per cent error for m = 9152 ranges from -2 per cent up to + 15.5 per cent. Near the singularity the values are worst as would be expected. A question that one might ask at this point: Is this discrepency near the boundary due to the proximity of the singularity or to the variable spacing or both? Two separate problems might be posed to answer this. One, with no singularity but with variable spacing; second, a singularity present but the spacing as near constant as stability conditions will allow.

It is felt that this method of combining the difference equations ("telescoping") holds considerable promise for variable coefficient parabolic partial differential equations since it can combine the higher accuracy of a fine mesh with the rapid progress of more coarse meshes once the coefficients have been calculated. Considerable experimenting was done with variable spacing and it seems that one should avoid using such spacing if possible. Various forms of the boundary conditions were tried other than a difference formulation and found to give much better results even with a singularity in the neighborhood.

The author is very grateful for the assistance of both Professor F. B. Hildebrand and Dr. F. M. Verzuh for their assistance, advice, and encouragement with this problem. Thanks should also go to the Statistical Services Staff of M.I.T. for their cooperation in the use of the CPC.

Philip L. Phipps

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Table I

	Difference		Equation	Coefficients		
n	h_n	x_n	J	$A_{n,J}$	$B_{n,J}$	$C_{n,J}$
-1	1	-1				
0	1	0	1	.375	.0	.625
1	2	1	1	.33333333	.375	.29166667
2	4	3	4	.5	.0	.5
3	8	7	8	.41666667	.125	.45833333
4	16	15	16	.375	.1875	.4375
5	32	31	32	.35416667	.21875	.42708333
6	64	63	64	.34375	.234375	.421875
7	128	127	64	.16927084	.62109375	.20963541
8	128	255	64	.18847656	.49804688	.31347656
9	128	383	64	.31347656	.24804688	.43847656
10	128	511	32	.21923828	.49902344	.28173828
11	128	639	32	.28173828	.37402344	.34423828
12	128	767	32	.34423828	.24902344	.40673828
N = 13	128	895	32	.40673828	.12402344	.46923828
14		1023				

Table II

Comparison of Analytic Steady State with Calculated Steady State

		(m = 4480, t = 1120)		(m = 8000, t = 2000)		(m = 9152, t = 2288)	
n	x_n	CPC calculated $U_{n,m}$	Values given by (11)	CPC calculated $U_{n,m}$	Values given by (11)	CPC calculated $U_{n,m}$	Values given by (11)
0	0	6.83198	5.88239	7.83198	6.86563	8.15396	7.18742
1	1	6.43666	5.47713	7.43664	6.46039	7.75862	6.78216
2	3	5.91561	4.96740	6.91549	5.95065	7.23747	6.27243
3	7	5.24955	4.38277	6.24919	5.36601	6.57117	5.68780
4	15	4.41031	3.75430	5.40941	4.73754	5.73137	5.05933
5	31	3.46331	3.10740	4.46130	4.09064	4.78324	4.41243
6	63	2.49642	2.46376	3.49230	3.44700	3.81420	3.76878
7	127	1.75301	1.84831	2.74515	2.83155	3.06699	3.15334
8	255	1.24094	1.30052	2.22718	2.28377	2.54892	2.60555
9	383	.99078	1.03847	1.97278	2.02170	2.29444	2.34350
10	511	.85256	.89382	1.83166	1.87765	2.15327	2.19884
11	639	.77625	.81358	1.75355	1.75355	2.07513	2.11861
12	767	.73921	.77413	1.71556	1.75737	2.03712	2.07916
13	895	.72927	.76284	1.70537	1.74608	2.02692	2.06786

EVALUATION OF THE EXPLICIT DIFFERENCE FORMULA FOR A PARABOLIC DIFFERENTIAL EQUATION

The introduction to the problem and a description of the procedures for optimization of the transient response have been given forth in Quarterly Progress Report No. 13, 14, and 15.

The optimum values of r_f and r for the $\Psi = 1$ case (case I) and the $\frac{\partial \Psi}{\partial x} = -1$ case (case II) were shown to vary around $R = \frac{1}{6}$, depending on the number of grid divisions, M. But for the $\Psi - Q\frac{\partial \Psi}{\partial x} = 1$ case (case III), the optimum values of r_f and r were found to be significantly lower than $\frac{1}{6}$ when Q is finite. The envelope R of the optimum values, when $M \to \infty$, for this case is shown in Figure 1.

The corner values $\Psi_{-1,0}$ and Ψ_{00}, defined in the earlier reports may be viewed as an initial impulse adjustment of magnitude A such that for case I

$$\Psi_{00} = A + f(0)$$

for case II $$\Psi_{-1,0} = \frac{2}{M}\left[A + f(0)\right]$$

and for case III $$\Psi_{-1,0} = \frac{2}{MQ_f}\left[A + f(0)\right]$$

where f(0) is the boundary input function at t = 0 which is 1 in the above cases. The initial impulse adjustment A is introduced to optimize the transient part of the response. The envelope of A_L, when $M \to \infty$, is shown in Figure 2. It is interesting to note that the A_L value approaches that for case I when $Q \to 0$ while on the other hand approaches that for case II when $Q \to \infty$.

Numerical experiments, aided by the Whirlwind Computer, show that the use of r value as defined by R in Figure 1 with the proper initial impulse adjustment imporves the transient response considerably when Q is finite. Improvement is optimum when r_f and r are differentiated described by the present procedures. For cases I and II the present procedures, however, yield no appreciable improvement over the use of $r_f = r = R = \frac{1}{6}$. For empirical guide on the choice of r and A values for cases under similar boundary conditions, Figures 1 and 2 are recommended.

Boundary input function of sin ωt, instead of a step, was also tried on the present procedures. Numerical results showed that the steady state error was dominant over the transient

error and improvement on the transient response had only minor effect on the overall response. It seems that the lower the r value chosen, the smaller would be the steady state error. But on the transient part of the response, this advantage may soon be somewhat offset by an increase in transient error.

For details of this work one may refer to a complete report with Professor S. H. Crandall of the Mechanical Engineering Department.

Andrew T. Ling

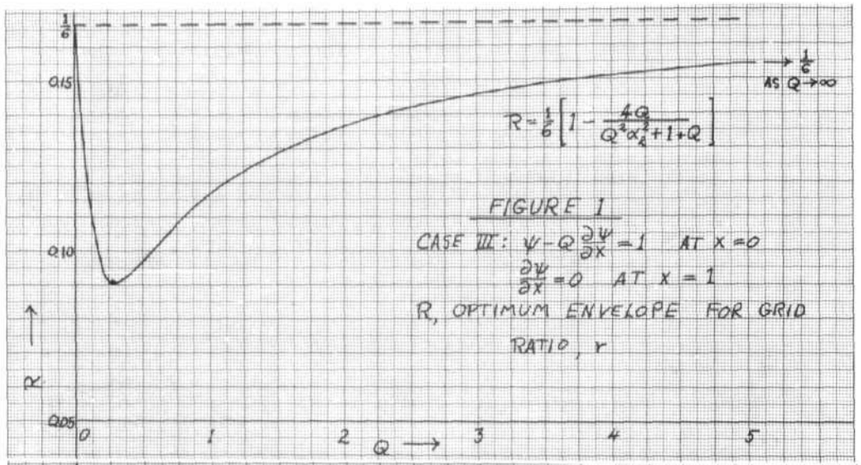

FIGURE 1

CASE III: $\psi - Q\frac{\partial\psi}{\partial x}=1$ AT $X=0$

$\frac{\partial\psi}{\partial x}=0$ AT $X=1$

R, OPTIMUM ENVELOPE FOR GRID RATIO, r

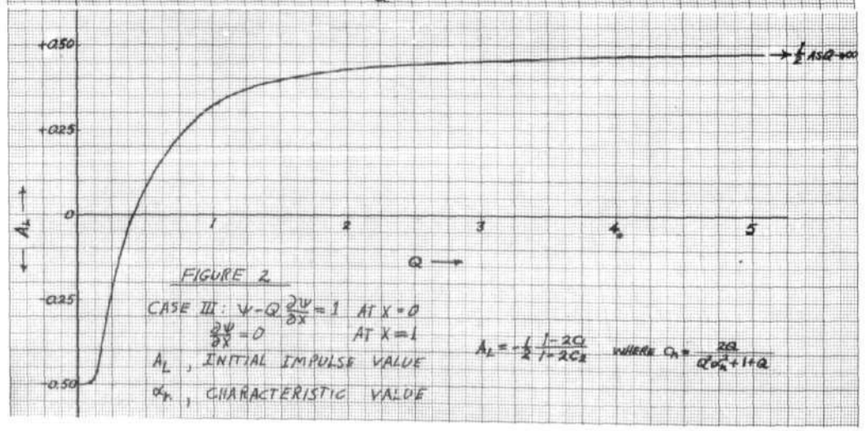

FIGURE 2

CASE III: $\psi - Q\frac{\partial\psi}{\partial x}=1$ AT $X=0$

$\frac{\partial\psi}{\partial x}=0$ AT $X=1$

$A_L = -\frac{1}{2}\frac{1-2Q}{1+2Q}$ WHERE $Q=\frac{2Q}{Q\alpha_1^2+1+Q}$

A_L, INITIAL IMPULSE VALUE

α_1, CHARACTERISTIC VALUE

STABILITY OF THIN, SHALLOW ELASTIC SHELLS

The general differential equations of shallow shell theory for a hyperboloidal shell are

(1) $$\nabla^2\nabla^2 F = Eh\left\{\frac{2c}{ab}\frac{\partial^2 w}{\partial x\partial y}+\left(\frac{\partial^2 w}{\partial x\partial y}\right)^2-\frac{\partial^2 w}{\partial x^2}\frac{\partial^2 w}{\partial y^2}\right\}$$

$$D\nabla^2\nabla^2 w = -p_o-\frac{2c}{ab}\frac{\partial^2 F}{\partial x\partial y}+\frac{\partial^2 w}{\partial x^2}\frac{\partial^2 F}{\partial y^2}+\frac{\partial^2 w}{\partial y^2}\frac{\partial^2 F}{\partial x^2}-2\frac{\partial^2 w}{\partial x\partial y}\frac{\partial^2 F}{\partial x\partial y}$$

where w is the deflection in the z-direction and F is the stress function. We will consider these equations under the following conditions

(a) The shell is uniformly loaded by p_o.

(b) The edges of the shell at x = 0, a and y = 0, b are assumed to have moment free support.

(c) The edge stiffeners of the shell are assumed to be rigid in the direction of their axes and to have negligible bending resistance in planes tangent to the shell.

Using these conditions, a solution of the Equations (1) is

(2) $$w = 0 \qquad F = -p_o\frac{ab}{2c}xy$$

To test the stability of this solution, we assume new solutions of the form

(3) $$w = 0 + \bar{w}\,, \quad F = -p_o\frac{ab}{2c}xy + \bar{\Phi}$$

substitute these into (1) and linearize the differential equations [1]. We then will consider two cases of the stability of the shell:

(A) We consider the edges of the shell to be "locked" in the displacements given by the linear membrane solution (2) and then we attempt to find the magnitude of the load, p_o, which causes buckling. That is, from (2) we may determine not only the deflection, w, but also the displacements, u and v, in the x and y directions by means of the stress-strain relations. Therefore, add to the conditions (a) - (c) the condition that, on the edges, u and v must be equal to the displacements derived from (2).

(B) We put no further restrictions on the shell. That is, in contrast to A, we allow u and v along the edges to vary from the linear membrane state, compatible with (c).

The boundary conditions corresponding to Case A are

(4) $$x = 0,a: \quad \bar{w} = \nabla^2\bar{w} = \bar{\Phi}_{xx} = \bar{\Phi}_{yy} = \bar{v} = 0$$
$$y = 0,b: \quad \bar{w} = \nabla^2\bar{w} = \bar{\Phi}_{xx} = \bar{\Phi}_{yy} = \bar{u} = 0$$

where analogously to (3) u and v are the deviations from the linear membrane state. The boundary conditions corresponding to Case B are precisely similar to those of Case A except that the restrictions on u and v are absent.

To find the buckling load, we assume series expansions for w and $\bar{\Phi}$, satisfying the boundary conditions, as follows:

(5) $$\bar{w} = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_{mn}\sin\frac{m\pi x}{a}\sin\frac{n\pi y}{b}$$
$$\bar{\Phi} = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} B_{mn}\sin\frac{m\pi x}{a}\sin\frac{n\pi y}{b} + B_{00}xy$$

Now in Case A the restrictions on the edge displacements effectively restrict the first derivatives of the stress function, $\bar{\Phi}$, through the stress-strain relations. For this reason we must have the $B_{00}xy$ in (5) for this term still enables us to satisfy the explicit boundary conditions on $\bar{\Phi}$ in (4) and at the same time makes it possible to satisfy the conditions on u and v. However, in Case B $\bar{\Phi}$ and its first derivatives are completely arbitrary on the edges so that we may without loss of generality take $B_{00} = 0$ in this case.

The boundary conditions of Case A make it convenient to express the problem in variational form [2]. Having done this, we substitute (5) into the variational expression, perform the integrations and take the variations and so end up with a doubly infinite plus one set of linear algebraic equations for the A_{mn}, B_{mn} and B_{00}.

In Case B the lack of restrictions on u and v make it inconvenient to use variational techniques. Instead we substitute (5) into the linearized differential quations for

w and $\bar{\phi}$ and then apply finite Fourier Transform techniques. Doing this, we get a doubly infinite set of linear algebraic equations in the A_{mn} and B_{mn}. These are identical with the equations for Case A except for those terms depending on B_{00}.

In either Case A or B we now have an infinite characteristic value problem to solve for the characteristic roots p_o. The smallest root gives us the buckling stress p_o. In order to solve the problem, we consider the series (5) terminated at finite values and solve the resulting finite characteristic value problem. We then investigate the convergence of the solution as we add more and more terms to the approximation. The form of the algebraic equations we have to deal with is

(6) $$Sx = p_o Hx$$

where S and S are symmetric matrices and S is positive definite. To solve this system when H and S are finite, we first reduce S to its canonical form and then diagonalize H. This amounts to the simultaneous reduction of two quadratic forms to sums of squares which may always be done if one of the matrices is positive definite [3]. Actually, the Equation (6) depends also on two parameters not explicitly shown:

(a) a/b the ratio of the linear dimensions

(b) h/c the ratio of shell thickness to shell rise

Computations are now under way on the Whirlwind I computer for various values of the parameters. Thus far no more than twelve terms have been used in the approximations and for values of h/c which are not too small this number of terms appears to give quite good convergence.

Anthony Ralston

References:

[1] Machine Methods of Computation and Numerical Analysis, Quarterly Progress Report No. 15, p. 12, March (1955).

[2] E. Reissner, Jour. Math. Phys. 32, Nos. 2, 3 (1953).

[3] A. Meckler, Quarterly Progress Report, Solid State and Molecular Theory Group, p. 15 October (1954).

STEEPEST DESCENT ANALYSIS OF RESISTIVITY DATA

It was found that many resistivity analyses attempted using the Newton Method gave unsatisfactoy results [1]. The error "surfaces" along which the iterations carry the solutions are generally non-linear enough to cause difficulty, usually extreme overshoot. It was necessary to compensate for this, during the first dozen or so iterations, by reducing the parameter changes made to about five per cent of that predicted. Only when very near the solution (fits better than one per cent at all kernel points) was it occasionally possible to use the entire prediction. Another unsatisfactory feature of the Newton solution was the necessity of solving a matrix to find the changes at each iteration. The matrix solution could introduce inaccuracy in a variety of ways (two variables nearly equal, giving degeneracy, or one variable orders of magnitude larger than another, or much closer to its solution). These conditions result in indeterminacy and wild predictions, or in singularity with the consequent machine difficulty.

Apparently the Newton method was not too well suited to the kinds of functions involved, and it decided to investigate the deepest descent solution for sets of non-linear algebraic equations. This is designed to use more data points than variables, giving a least-square fit. It does not require solving a matrix. In addition, a way was found to compensate to a certain extent for the large differences in magnitude of the variables, a result of their dimensional disparity (ρ = resistivity, d = length). This procedure was found superior to the Newton procedure and is described below.

Reconciling the notation of the previous report with that of Householder:

$$\psi_i = f_3(\lambda_i) - F(\lambda_i) \equiv f_{3i} - F_i$$
$$f_{3i} = \frac{1}{1+k_{3i}} - \frac{1}{2} = \frac{u_{i+2}\, t_i}{2}$$
$$F_i \equiv \frac{1}{1+K_i} - \frac{1}{2}$$
$$\Phi = \sum \psi_i^2 = \sum_i (f_{3i} - F_i)^2$$
$$x_s(\xi_i) = x_i^{(s)} \quad \text{, (result of } s \text{ iterations)}$$

Proceeding with Householder's notation

$$x_1 = x_0 - \lambda u$$

and, in general

$$x_{s+1} = x_s - \lambda_s u_s$$
$$(\xi_i)_{s+1} = \xi_i - \lambda_s (u_s)_i$$

where

$$u_s = (\nabla \phi)_s$$
$$(u_s)_i = (\nabla \Phi_i)_s$$

the i^{th} components of $\nabla\varphi$ after s iterations, and λ is such as to minimize φ. In particular, for a three-layer case, ρ_1 and ρ_3 known, $\xi_1 = \rho_2$, $\xi_2 = d_2$, $\xi_3 = d_1$

$$\nabla\Phi_i = (\partial\Phi/\partial\xi_i) \Big/ \left[\sum_i (\partial\Phi/\partial\xi_i)^2\right]^{1/2}$$
$$\nabla\Phi_1 = (\partial\Phi/\partial\rho_2) \Big/ \left[(\partial\Phi/\partial\rho_2)^2 + (\partial\Phi/\partial d_2)^2 + (\partial\Phi/\partial d_1)^2\right]^{1/2}$$

As mentioned previously, the dimensional disparity of the unknowns results in some of the u_i being much larger than others. This, in turn, causes the variables with smaller derivatives to be relatively ignored in the iterations until those with larger derivatives are very nearly at a minimum. Such is the case when the second layer is thin and very resistive--the resistivity is virtually ignored until the end of the solution. Compensation can be achieved by using, instead of the u_i given above,

$$u_i = \frac{\xi_i \frac{\partial\varphi}{\partial\xi_i}}{\left[\sum_i \left(\xi_i \frac{\partial\varphi}{\partial\xi_i}\right)^2\right]^{1/2}}$$

This worked satisfactorily.

The optimum value of λ can be found exactly only by trial and error. For any function, G, it can be approximated by $\frac{G}{G'}$, or $\frac{G'}{G''}$, etc., each successive approximation being exact for a higher order power series (Newton approximation). However, if the function is not expressible in a power series expansion, then the approximations are not necessarily valid, and successive Newton approximations may become poorer. Such, for instance, is the case when non-integral powers appear in the function.

Examination of the error surfaces showed that negative second derivatives were not uncommon when at some distance from the minimum. Near the minimum, however, curvature is always upward. The calculation of λ was handled as follows. From the first estimates, $x_o(\xi_1, \xi_2, \xi_3)$, the function φ_o was calculated, as were

$$\phi_o' = \sum_i \frac{\partial\phi}{\partial\xi_i}\frac{d\xi_i}{ds}$$

and

$$\phi_o'' = \sum_i \frac{\partial^2\varphi}{\partial\xi_i^2}\left(\frac{d\xi_i}{ds}\right)^2$$

the first and second derivatives of φ_o along the gradient path. Then new trial values, Θ, of φ were calculated from

$$\theta_1 = x_o - c_1(\phi_o'/\phi_o'')u_o$$
$$\theta_2 = x_o - c_2(\phi_o'/\phi_o'')u_o$$

---

[1] Obviously $\frac{G}{G'}$ is exact for a linear function, and $\frac{G'}{G''}$ for a parabolic function. There is a difference between these two approximations that is of considerable importance when the error surface, as here, does not go to zero because of errors in the data. It is seen that a linear extrapolation used under these conditions will always overshoot.

such that

$$\Theta_1 = \Theta(\gamma_1).$$

A value of c was then found by interpolation which would minimize Θ. Because of the behavior of the error curves, the value c could not be obtained in the same manner when near the solution as when at some distance away. It was found best to use a linear interpolation to $\Theta = 0$ at the beginning of the calculations, and a parabolic interpolation to Θ = minimum at the end. That is, near the beginning, assume

$$\theta_j = c_j\alpha + \beta$$

and use

$$c = -\frac{\beta}{\alpha} = -\frac{\theta_1 - \theta_2}{c_1 - c_2}$$

at the end, assume

$$\theta_j = c_j^2\alpha + c_j\beta + \gamma$$

and use

$$0 = 2\alpha c + \beta$$

$$c = -\frac{\beta}{2\alpha} = -\frac{c_1^2(\theta_2 - \theta_3) + c_2^2(\theta_3 - \theta_1) + c_3^2(\theta_1 - \theta_2)}{\theta_1(c_2 - c_3) + \theta_2(c_3 - c_1) + \theta_3(c_1 - c_2)}$$

changing from linear to parabolic when

$$a_3 \leq |\theta_1 - \theta_2|.$$

In the cases analyzed, values of c have generally been between 1/2 and 3/2.

Proceeding with the iteration then,

$$\lambda_o = c\frac{\phi_o'}{\phi_o''}$$

$$x_1 = x_o - \lambda_o u_o \quad , \text{etc.}$$

When this work was begun, it was felt that such an "interpolation within an interpolation" procedure might be inefficient because of the two "dummy" iterations for every true iteration. In practice this has not proved the case, since errors diminish at four to five times the rate of the ordinary steepest descent procedure on the same data. For more regular error surfaces, of course, it is probable that only one kind of interpolation (linear or parabolic) would be satisfactory.

Results

Most cases analyzed here were those in which difficulty was encountered in the Newton analysis, (Vozoff 1955). In addition, two other "difficult" cases and two of the field cases were re-analyzed. Comparison of cases 5, 6, 10, and 11 with the results of the Newton analysis shows the greater power of the Steepest Descent analysis to reduce the error of the solution. However, it will be noted that the solutions in the two field cases, B and C, are not significantly different from the Newton solutions as might be expected. The thick second layers make them "easy" cases.

Cases 10a and 10b show the results of some of the more common Steepest Descent procedures on the data of case 10. Both use the non-normalized u_{10}. Case 10a was done changing one parameter at a time. Case 10b was solved changing all parameters simultaneously, differing from the rest of the analyses only in the non-normalized u_1. Both methods are slower than the normalized gradient group descent.

Conclusions

The normalized gradient group descent analysis presented here possesses two advantages over other methods used for the resistivity problem. First, by virtue of its Steepest Descent nature, it has a better chance of converging to a solution than does the Newton method. Second, the normalization and type of interpolation used allow more rapid convergence to a solution than do the standard Steepest Descent techniques.

This technique probably should be applied to cases of more than three layers.

It is again a pleasure to acknowledge the advice of T. R. Madden.

Keeva Vozoff

Reference:
[1] Machine Methods of Computation and Numerical Analysis, Quarterly Progress Report No. 15, p. 33, March (1955).

Three-Layer Analysis of Three-Layer Kernels

Case	True Values ρ_1 / d_1	ρ_2 / d_2	ρ_3	$d_2\rho_2$ / d_2/ρ_2	Solution ρ_1 / d_1	ρ_2 / d_2	ρ_3 / ϕ	$d_2\rho_2$ / d_2/ρ_2	A++
5	1.	.05	5.		1.	.101	5.		
	1.	.5		10.	.902	1.01	$9.\times10^{-9}$	10.	3
6	1.	10.	.2	5.0	1.	4.26	.2	5.11	3
	1.	.5			.923	1.20	$5.\times10^{-7}$		
10	1.	10.	.1	1.	1.	1.42	.1	1.27	3
	1.	.1			.742	.893	1.7×10^{-7}		
10a	1.	10.	.1	1.	1.	19.3	.1		3
	1.	.1			.987	.0524	$7.\times10^{-7}$		
10b	1.	10.	.1	1.	1.	19.6	.1		3
	1.	.1			1.22	.0443	$9.\times10^{-5}$		
11	1.	10.	.2	1.	1.	19.5	.2	1.01	3
	1.	.1			.988	.0516	$6.\times10^{-7}$		
26a	1.	.05	5.		1.	.514	5.		4
	1.	.01		.2	1.87	-.33	$3.\times10^{-6}$		
26b	1.	.05	5.		1.	.517	5.		6
	1.	.01		.2	1.87	-.34	2.6×10^{-6}		
27	1.	.1	5.		1.	.120	5.		6
	1.	.01		.1	.930	.0198	$3.\times10^{-8}$	.165	

++ This column indicates number of places accuracy of kernel used.

Three-Layer Analysis of Field Kernels

Case	First Estimate			Solution		
	P_1	P_2	P_3	P_1	P_2	P_3
	d_1	d_2	φ_0	d_1	d_2	φ
B	1.	.6	.2	1.	.929	.2
	.15	3.	$3.\times10^{-4}$	.174	2.72	1.3×10^{-5}
C	1.	.25	.2101	1.	.251	.2101
	.3	6.	3.3×10^{-4}	.272	5.97	1.7×10^{-4}

3. ACADEMIC PROGRAM

3.1 Institute Courses and Seminars

COURSES ON DIGITAL COMPUTER CODING AND LOGIC

Course 6.535, Introduction to Digital Computer Coding and Logic, a discussion of selected topics in programming, logical design and applications of large scale digital computers, was offered by D. Arden at MIT during the spring of 1955. The course included the solution of a programming problem on a simplified single address computer simulated by Whirlwind I. Among the problems solved by the class members were the solution of simultaneous linear equations, integration of differential equations, and the economization of power series. The total enrollment was 55 seniors and graduate students (from both the engineering and industrial management curricula).

The Digital Computer Laboratory Comprehensive System (CS II) programming course was given once during this quarter. The course includes the following topics: relative addresses, temporary storage, floating addresses, preset parameters, programmed arithmetic, cycle counters, buffer storage, automatic output, post mortems, and multipass conversion. The text for the course is a programmer's manual written by staff members of the S and EC Group. The 26 students enrolled during this quarter represented the following groups: Department of Business and Engineering Administration, School of Industrial Management, Department of Nuclear Engineering, Spectroscopy Laboratory, Laboratory for Nuclear Science, Naval Supersonic Laboratory, Chemical Engineering Department, Physics Department, Solid State and Molecular Theory Group, Aeronautical Engineering Department and Lincoln Laboratory.

NUMERICAL ANALYSIS

This year, for the first time, Professor Hildebrand gave a second semester course in Numerical Analysis, M412. This semester the context of the course was made up of the following topics: Least-squares approximation, smoothing of data, quadrature formulas of Gauss and Chebyshev types, harmonic analysis, exponential and trigonometric approximation, determination of periodicities, Chebyshev approximation, continued fraction expansions and rational-function approximation, numerical solution of partial differential equations.

MACHINE METHODS OF COMPUTATION AND NUMERICAL ANALYSIS

During the last quarter the biweekly seminars for the project reported in Part I were completed and brought to a close for the academic year. The high points for the quarter were two lectures presented by guests from the National Bureau of Standards and two lectures jointly presented by the Meteorology Department and the Mathematics Department of MIT.

The guest lecturers were Dr. Milton Abramowitz and Dr. Franz Alt. Dr. Abramowitz spoke on "Coulomb Wave Functions", a topic which is important to the physicists of the project, as one can tell by referring to the comments on Group Activities prepared for the previous progress report. Dr. Alt spoke about the type of problems which as yet present overwhelming difficulties (storage demands, etc.) for the modern electronic computer.

The joint lectures by the Meteorology and Mathematics Departments brought results which are summarized in the report entitled: "Multiple Prediction" (Part I, Section 2.2 above). These lectures presented the multiple prediction techniques currently being applied by the MIT Meteorology Department as well as the Matrix Factorization work of Professor Wiener which should lead to a scalar solution of the multiple prediction problem. These two points of view (cf. problem 155, Part II, Section 2.2 and reference [3] of Multiple Prediction) revealed the need and potential availability of a scalar solution to weather prediction in the multiple series case that has previously been available only for single series. It seemed profitable to look into the matter further and this was done during some meetings of the probability seminar of the mathematics department, the numerical analysis discussion group of the project (see Section 3.2 below) and during further conversations with Professor Wiener.

3.2 Group Activities

NUMERICAL ANALYSIS DISCUSSION GROUP

The usual membership and purpose of this group have been recorded in previous reports. The majority of the discussions during the last quarter were held for the purpose of obtaining the multiple prediction solution (see Part I, Section 2.2 and Section 3.1 above) and consequently were attended mainly by Professor Armand Siegel, Physics Department, Boston University, Dr. Joseph G. Bryan, DIC Staff at MIT, Mr. Peter Hanna and Mr. Robert Miller,

ACADEMIC PROGRAM

Meteorology Department, MIT and Dr. Bayard Rankin, Mathematics Department, MIT.

COULOMB WAVE FUNCTIONS

The programming of Coulomb Wave Functions, being carried out jointly by some physics department members of the Committee on Machine Methods of Computation, is still in progress.

NUMERICAL ANALYSIS LABORATORY

The supervision of the Numerical Analysis Laboratory, which is open approximately 8 hours a week in conjunction with Professor Hildebrand's course M412, and the grading of homework problems has been done by M. Douglas McIlroy, Philip M. Phipps,and Anthony Ralston.

PART II

Project Whirlwind

1. REVIEW AND PROBLEM INDEX

This report covers the specific period of March 21, 1955 to June 13, 1955. During this time 74 problems made use of 332.8 hours of the 546.5 hours of Whirlwind I computer time allocated to the Scientific and Engineering Computation (S and EC) Group. The remaining 213.7 hours of the allocated time were used for terminal equipment testing and calibration, demonstrations, tape conversions for Lincoln Laboratory, and various inter-run operations not logged to specific problems.

These problems cover some 18 different fields of applications. The results of 27 of the problems have been or will be included in academic theses. Of these, 19 represent doctorate theses, 3 engineering, 7 master's, and one bachelor's. Thirty-three of the problems have originated from research projects sponsored at MIT by the Office of Naval Research.

Two tables are provided as an index to the problems for which progress reports have been submitted. The first table arranges the problems according to the field of application indicating the source of each problem and the per cent of the WWI machine time consumed. The second table attempts to arrange the reports according to the principal mathematical problem involved in each. In each table letters have been added to the problem number to indicate whether the problem is for academic credit and whether the problem is sponsored.

It may be seen from table 2-I that problems originating from ONR sponsored research used 60.61 per cent of the total WWI problem time. This 60.61 per cent includes 11.78 per cent used by the Digital Computer Laboratory staff, 9.67 per cent used by the Solid State and Molecular Theory Group, and 21.30 per cent by the Machine Methods of Computation Group.

A Data Reduction Symposium was sponsored at the Digital Computer Laboratory by the Servomechanisms Laboratory. A report on this symposium is included under Problem 126.

A routine that computes and displays some 15,000 five-digit numbers on 145 frames in about four and one-half minutes was used in Problem 224.

The Whirlwind programmed-marginal checking facilities have been expanded to include additional terminal equipment.

Reliability figures are provided for the Whirlwind computer system covering the 33-week period beginning on 28 September 1954. During this period, the average uninterrupted operating time between failure incidents was 10.8 hours.

PROBLEM INDEX

Field	Description	Problem Number	WWI Time	Source
Aeronautical Engineering	Transient response of aircraft structures to periodic air loading	254 C.	.85	MIT
	Horizontal stabilizer analysis	255 C.	.97	MIT
	Horizontal stabilizer modes, shapes and frequencies	257 C.	.46	MIT
	Helicopter rotor blading data units	260 B.	1.18	MIT
Business and Eng. Administration	Numerically controlled slitting machine routine loads	267 B.	.65	MIT
Chemical Engineering	Reactor runaway prevention	* 231 B,N.	.09	MIT
	Transients in distillation columns	241 B,N.	1.51	MIT
	Calculations for the MIT reactor	250 A.	2.51	MIT
	Critical mass calculations for cylindrical geometry	270 B.	1.00	MIT
Civil Engineering	Response of a five story frame building under dynamic loading	* 235 C.	.46	MIT
	Dynamic analysis of bridges	247 C.	2.45	MIT
	Analysis of two story steel frame building	* 258 N.	1.02	MIT
	Dynamic behavior of shear wall resting mobile	* 264 D.	.40	MIT
	Dynamic buckling	241 B.	.05	MIT
Dynamic Analysis and Control Laboratory, Electrical Engineering	Dynamic analysis of an aircraft interception	258 C.	1.71	MIT
	Optimization of alternator control system	264 C.	.57	MIT
	Extrapolation techniques	268 B.	.21	MIT
	Evaluation of a gear profiling technique	271 B.	.07	MIT
Geology and Geophysics	Geophysical data analysis	104 C.	.52	MIT
	Earth resistivity interpretation	* 123 B,N.	1.00	MIT
	Dispersion curves for seismic waves, multilayered media	* 218 B,N.	1.73	MIT
	Fourier synthesis for crystal structures	261 C.	1.52	MIT
Instrumentation Laboratory	Distance and control	253 C.	1.34	MIT
	Flight path of an aircraft during curing	253 C.	1.17	MIT
	Response of the human pilot in a jet supersonic fighter flying a least pursuit course	256 B.	.05	MIT
Lincoln Laboratory	Evaluation of the reflection coefficient in a semi-infinite rectangular wave guide	150 L.	.04	MIT
	Eigenvalue problem in the propagation of electromagnetic waves	1st D.	1.04	MIT
	Ionosphere constants	214 L.	.08	MIT
	General regular solution	272 L.	.30	MIT
Mathematics Department	Number of structures of relations on finite set	* 242 N.	.07	MIT
	Buckling of shallow elastic shells	* 27 B.	2.11	MIT
Mechanical Engineering	Flow of compressible fluids (aerothermopressor)	120 B,N.	5.40	MIT
	Laminar boundary layer of a steady, incompressible flow in the entrance region of a tube	124 N.	.89	MIT
	Industrial process control studies	129 B.	.48	MIT
	Evaluation of difference diffusion equation	* 229 N.	.53	MIT
	Correlations and transforms	283 C.	.30	MIT
	Rolling bearings	247 C.	.20	MIT
Meteorology Department	Synoptic climatology	156 N.	6.45	MIT
	Computations of the fields of vertical velocity and horizontal divergence	224 N.	4.20	MIT
	Investigation of the vorticity field in the general circulation of the atmosphere	226 D.	.61	MIT
	Surface pressure prediction	247 C.	1.25	MIT
	Correlation function	280 B.	1.57	MIT
Naval Supersonic Laboratory	Heat transfer through high-speed laminar boundary layers	284 C.	.38	MIT
	Wind tunnel data reduction	248 C.	.12	MIT
Operations Research Group	Information handling in task groups	265 B.	.35	MIT
Physics Department	Slaters wave functions	* 122 N.	1.25	MIT
	Self-consistent molecular orbital	144 N.	.28	MIT
	Overlap integrals of molecular and crystal inquire	* 178 B,N.	5.26	MIT
	An a-gented plane wave method as applied to sodium	194 B,N.	0.52	MIT
	Exchange integrals between real Slater orbitals	204 N.	.33	Univ of Chicago
	Variation-perturnation of atomic wave function and energies	* 210 N.	.96	MIT
	Transformation of integrals for diatomic molecules	210 N.	.25	MIT
	Neutron-deuteron scattering	* 225 B,N.	.98	MIT
	Eigenvalues for a spheroidal square well	* 236 B,N.	8.03	MIT
	Self-consistent calculation of nuclear mass density	* 236 B,N.	4.96	MIT
	Theory of electron reactions	245 B.	3.08	MIT
	Scattering from oxygen	* 260 B,N.	.14	MIT
	Energy levels of diatomic hydrides	260 N.	1.04	MIT
	Electron diffusion in an electromagnetic field	262 N.	1.03	MIT
	Analysis of air shower data	273 N.	.07	MIT
	Multiple scattering of waves from a spatial array of spherical scatterers	274 N.	.61	MIT
	Energy levels of diatomic hydrides LiH	276 N.	.38	MIT
	Augmented plane wave method as applied to cuprous crystal	285 N.	.79	MIT
	Atomic wave functions	286 N.	.37	MIT
	Polarizability effects in atoms and molecules	290 N.	.06	MIT
Servomechanisms Laboratory	Data reduction program, polynomial fitting	126 C.	1.78	MIT
	Subroutines for the numerically controlled milling machine	142 D.	.48	MIT
	Translator program for the numerically controlled milling machine	260 C.	.70	MIT
Miscellaneous	Comprehensive system of service routines	100.	9.15	MIT
	Special problems (staff training, demonstrations, etc.)	151.	1.00	MIT
	G and EC subroutine study	191.	.66	MIT
	Informal routines	195 C.	1.30	Mass. Memorial
	Unlisted 1 + SRA 1103 translation program	266 C.	8.32	MIT
	Course 6.251, Spring 1959, Practice	292 A.	3.57	MIT

Table 2-I Current Problems Arranged According to Field of Application
(* MIT Project on Machine Methods of Computation)

Mathematical Problem	Procedure	Problem Number
1. Matrix algebra and equations		
Matrix multiplication, addition, diagonalization	Basic operations	144 N.
Zeros of a matrix equation	Interpolation	* 212 B,N.
Minimize an analytic equation	Basic arithmetic operations	* 213 N.
Orthonormalization	Schmidt process	215 N.
Root of a determinantal equation	Iteration	266 A.
Linear equations	Crout's method	270 B.
Eigenvalues	Iteration	* 270 B.
Simultaneous equations	Iteration	277 C.
Eigenvalues	Diagonalization	278 N.
Matrix inversion	Crout's method	285 B.
Eigenvalues	Diagonalization	286 N.
Eigenvalues	Diagonalization	288 N.
Orthonormalization, Eigenvalues	Schmidt process, diagonalization	290 N.
2. Ordinary differential equations		
Seven nonlinear first order system	Fourth-order Runge-Kutta	120 B,N.
Five nonlinear second order	Gill's method	199 N.
Second order linear	Difference equation	* 205 C.
Set of first order	Difference equation	230 C.
Set of nonlinear first order	Gill's method	234 C.
Wave equation	Second order Runge-Kutta	241 B,N.
Nonlinear second order	Milne predictor-corrector formula	245 N.
Set of eight first order	Finite differences	* 252 N.
Five equations with 30 sets of initial conditions	Gill's method	258 C.
Different sets of ordinary differential	Gill's method	263 C.
Second order nonlinear ordinary differential	Step-by-step	267 C.
Second order differentials	Kutta-Gill	269 L.
System of three equations	Kutta-Gill	* 269 D.
Second order	Runge-Kutta-Gill	282 B.
Twenty-five simultaneous equations	Gauss-Jackson method	285 N.
System of ordinary differential	Runge-Kutta	290 B.
	Difference equations	291 B.
3. Partial differential equations		
Schroedinger's equation	Sumation of series	* 122 N.
Diffusion equation	Recurrence formula	* 228 N.
Schroedinger's equation in spherical coordinates with non-reparable potential	Matching wave functions at the boundary	* 235 B,N.
Second order parabolic	Explicit finite differences	256 C.
First order system	Finite differences	224 N.
First order system	Finite differences	226 D.
4. Integration		
Integral evaluation	Trapezoidal rule	* 123 B,N.
Complex integral evaluation	Trapezoidal rule	156 L.
Overlap integrals	Evaluation of analytic forms	* 172 B,N.
Autocorrelation and Fourier transform	Simpson's rule	195 C.
Integral evaluation	Gaussian quadrature	204 N.
Auto- and crosscorrelation	Simpson's rule	213 D.
Stationary point of a variational	Simpson's rule	* 225 B,N.
Hartree-Fock equations	Trapezoidal plus variational	* 258 B,N.
Overlap integrals	Evaluation of analytic forms	260 N.
Evaluation of integrals	Approximation by algebraic functions	* 266 B,N.
Integration	Simpson's rule	278 N.
Integral evaluation	Trapezoidal rule	289 C.
Overlap integrals	Evaluation of analytic forms, Simpson's rule	290 N.
5. Statistics		
Multiple time series	Prediction by linear operators	106 C.
Calculation of the coefficients of a multiple regression system	Inner products	155 N.
Numerical prediction	Quadratic approximation	247 C.
Multiple time series	Correlations, means, frequency distribution	259 L.
Maximum likelihood estimation	Means, weighted sums, etc.	271 B.
Multiple time series	Correlation and transforms	280 B.
Multiple time series	Correlation and transforms	281 C.
6. Transcendental equations		
System of 47 equations	Step-by-step	* 251 B,N.
Nonlinear equations	Steepest descent	264 C.
System of nonlinear equations	Iteration	272 L.
Curve fitting	Least squares	273 N.
Nonlinear system of equations	Steepest descent	293 C.
7. Data reduction		
General data reduction	Polynomial fitting, etc.	126 C.
Surface fitting	Polynomial fitting, etc.	267 B.
Extrapolation and prediction	Least squares	268 B.
Function evaluation	Arithmetic operations	294 C.
8. Group theory		
Generation of projection operators	Machine generation	194 B,N.
Nonisomorphic relations on a finite set	Direct evaluation	* 242 N.
9. Complex algebra		
Complex roots and function evaluation	Iteration	193 L.
10. Fourier series		
Fourier synthesis	Direct evaluation	261 C.
Summing series	Direct evaluation	274 N.

Table 2-II Current Problems Arranged According to the Mathematics Involved
(* MIT Project on Machine Methods of Computation)

2. WHIRLWIND CODING AND APPLICATIONS

2.1 Introduction

Progress reports as submitted by the various programmers are presented in numerical order in Section 2.2. Since this summary report presents the combined efforts of DIC Projects 6345 and 6915, reports on problems undertaken by members of the Machine Methods of Computation Group have been omitted from Section 2.2 of Part II to avoid duplication of Part I. Suitable cross reference has been included in Section 2.2 of Part II for completeness.

Of the 74 problems described below, thirty-one (226, 258, 259, 264-266, 267-275, 277, 278, 280-283, 286, 290-294) represent new problems that are being described for the first time. Eleven problems (224, 230, 238, 247, 263, 268, 282, 283, 286, 292 and 294) have been completed.

Tables 2-I and 2-II have been set up to provide the reader with a convenient index to various interesting aspects of the problems. Table 2-I lists the problems according to their fields of application and indicates the source of each problem and the percent of the S and EC Group's Wwl problem time (332.8 hours) used by each. The mathematical problems and procedures involved in the various current problems are tabulated separately in Table 2-II. In both tables, problem numbers prefixed by asterisks (*) represent work being performed by members of the Machine Methods of Computation Group.

Letters have been added to the problem numbers to indicate whether the problem is for academic credit and whether it is sponsored. The letters have the following significance:

A implies the problem is NOT for academic credit, is UNsponsored.

B implies the problem IS for academic credit, is UNsponsored.

C implies the problem is NOT for academic credit, IS sponsored.

D implies the problem IS for academic credit, IS sponsored.

N implies the problem is sponsored by the ONR.

L implies the problem is sponsored by Lincoln Laboratory.

The absence of a letter indicates that the problem originated within the S and EC Group.

A section on Systems Engineering has been included in the Appendix of this Summary Report. This section was omitted from Summary Report No. 41 since it does not represent work being carried out under the present contract. However, because of its general interest and obvious relationship with the general use of the computer, this section will be included in this and succeeding reports.

2.2 Problems Being Solved

100. COMPREHENSIVE SYSTEM OF SERVICE ROUTINES

The Director Tape Program

A drastic revision of the director tape program is being made in order to remove several known errors and to make the entire system more useful.

One drawback of the present system of director tapes is that in a large number of cases the performance request is affected by whether or not a director tape will be used. In particular, a programmer may alter the final control block of a binary tape so that the computer is not stopped after read-in but instead begins the computation; or a programmer may terminate his program by reading in the next program instead of stopping the computer. If a director tape is not being used, the programmer can omit the instruction, rs (press restart button), from the performance request in the first case, and the instruction, ri (press read-in button), in the second case. If a director tape is being used, both words must be included.

The present version of the director tape program is being modified so that the performance requests in both of the above cases will be the same.

The following new words are being added to the director tape vocabulary:

(1) si 1 switch on,

(2) si 1 switch off,

The function of these words will be to set an indicator request on the buffer drum.

The utility control program will be modified so that the following will occur after a binary tape or a CS flexo tape has been read-in under director tape control.

If the si 1 switch indicator is set to "on", then computer control will be transferred to the director tape program which will look for a new director word.

If the si 1 switch indicator is set to "off", then computer control will be transferred immediately to the program just read in.

Recording of Flad Table on the Buffer Drum

The CS conversion program has been modified so that the table of floating addresses is left recorded on group 2 of the buffer drum after each conversion.

This step will facilitate the writing of post-mortem programs in which instructions can be printed out with symbolic addresses.

106 C. MIT SEISMIC PROJECT

As discussed in various previous reports, Problem 106 is concerned with the investigation of the use of statistical analysis techniques in seismic record interpretations, and, in particular, in the separation of "reflections" from background interference on these records. More complete descriptions of the problem and the approaches used are contained in "Detection of Reflections on Seismic Records by Linear Operators".1.

The reader is referred to Summary Report No. 41 for the more recent approaches to the problem. The program now being developed is a direct spectral factorization program, yielding 50 terms of the minimum phase impulse response.

Research reports are sent to a restricted group of supporting companies, but reproductions may be obtained through the special collection division of the MIT Hayden Library, six months after the reports are sent to the companies.

The programmers for this problem are S. Simpson, D. Grine, S. Treitel, and I. Calnan of the MIT Department of Geology and Geophysics.

S.M.Simpson, Jr.
Geology and Geophysics

Reference

1. Wadsworth, Robinson, Bryan, and Hurley --GEOPHYSICS, Vol. 18, No. 3, July 1953

120 B,N. THERMODYNAMIC AND DYNAMIC EFFECTS OF WATER INJECTION INTO HIGH-TEMPERATURE, HIGH-VELOCITY GAS STREAMS

This problem is connected with the development of a potential gas turbine component, called an "Aerothermopressor", in which a net rise in stagnation pressure of a hot gas stream is brought about by the evaporation of liquid water injected into a high-velocity region of the flow. The concepts underlying the operation of the Aerothermopressor are an outgrowth of comparatively recent work in the field of gas dynamics, and its proposed function in the gas turbine cycle is analogous to that of the condenser in a steam power plant.

The device consists of a converging nozzle which accelerates the exhaust gases from the turbine into a circular duct of varying diameter terminated by a conventional conical diffuser, which recovers the kinetic energy of the flow before discharging it to the atmosphere. At the entrance of the duct, special injectors deliver minute jets of water which are in turn atomized by the rapidly moving gas stream.

The changes in state within the Aerothermopressor are brought about by the simultaneous thermodynamic and dynamic effects of (a) evaporation of the liquid water, (b) momentum and energy interactions between the phases, (c) friction, and (d) variations in cross-sectional area of the duct. Under proper circumstances, these effects bring about a net rise in stagnation pressure across the device. Further descriptions of this device may be found in earlier reports, beginning with Summary Report No. 32, Fourth Quarter, 1952.

The role of Whirlwind I in the successful development of the Aerothermopressor is intimately connected with the determination of performance characteristics of the device

under all conditions of operation by means of a comprehensive one-dimensional analysis of the process. This analysis involves the simultaneous solution of seven, nonlinear, first-order differential equations.

During the past quarter, computations were resumed using a new Whirlwind program (see preceding Summary Report). These computations were divided into two categories: (a) those devoted specifically to studies of Aerothermopressor performance, and (b) those connected with further testing of the program and with studies of the various methods of numerical analysis which it contains.

To illustrate the flexibility of the program, a typical calculation falling within category (a) above will be briefly described. The problem was to calculate the supersonic critical performance of an Aerothermopressor consisting of an 11" diameter shell, seven feet in length and terminating in a conical diffuser having an included angle of five degrees. Within the outer duct and beginning five inches from its entrance, an axially-symmetric plug, having a parabolic diameter variation from zero at its nose to a maximum of 4.41-inches three-and-one-half feet downstream of the hose, was to lie along the axis of symmetry of the duct. A normal shock from supersonic to subsonic flow was desired 51-inches downstream of the duct entrance. The sequence of calculations were fully automatic and included provision for varying the increment size to keep truncation error within a reasonable bound. The singular solution (critical) was automatically determined by an iterative procedure which adjusted the initial Mach Number until a transition from subsonic to supersonic flow at constant area could be accomplished. One foot from the duct entrance, the calculation of liquid temperature was automatically modified to prevent later oscillation in this function. These calculations used the second-order Runge-Kutta method and required about twenty minutes of computer time.

In the category of further testing of the new program, a routine was written for accurately timing the calculations using the Whirlwind clock. The results are summarized below:

NUMERICAL METHOD	TIME PER INCREMENT, IN SECONDS	APPROXIMATE TIME PER INCREMENT FOR OLD PROGRAM, IN SECONDS
Euler, First-order	0.96	4
Backward differences, first-order	0.98	-
Runge-Kutta, second-order	1.83	-
Runge-Kutta, fourth-order	3.56	15
Forward and Successive differences (three-point formulas)	2.68	-
Wet-bulb temperature calculation	0.2	8

These comparative results between the new program and the earlier one provide an excellent example of the saving in computer time that can be realized with elimination of interpretive programming whenever possible. The new program is nominally four times as fast, and when the wet-bulb calculation routine is required, it is about six times as fast (for the fourth-order Runge-Kutta case). It should be pointed out that the significant reduction in the wet-bulb calculation time is due partly to a complete revision of the method of calculation.

Numerical analysis studies have been initiated in an effort to determine the most favorable increment size and numerical method from the point of view of keeping the computational time to a minimum while also maintaining adequate accuracy. These studies involve a computation of the stream properties over a given interval using a variety of increment sizes and then extrapolating to zero increment size for the 'exact' solution. Due to time limitations for this sort of study, results have been obtained thus far only for the "starting" regime of the calculations, which has arbitrarily been taken as 0.01 foot. A portion of the results for a particular case are summarized below:

(All quantities refer to stagnation pressure ratio, p_o/p_{o1}, at Z = 0.01 feet)

NUMERICAL METHOD	ACCUMULATED ERROR	INCREMENT SIZE	NO. OF STEPS	TIME OF COMPUTATION
	o/o	feet	*	seconds
Euler	0.073	0.00028	35.7	34.2
2nd-order Runge-Kutta	"	0.00140	7.15	13.1
4th-order Runge-Kutta	"	0.00213	8.23	29.4
Euler	0.28	0.00081	12.32	11.8
2nd-order Runge-Kutta	"	0.00249	4.01	7.3
4th-order Runge-Kutta	"	0.00351	2.85	10.2
Euler	0.70	0.00162	6.16	5.9
2nd-order Runge-Kutta	"	0.00371	2.70	4.9
4th-order Runge-Kutta	"	0.00490	2.04	7.3
Euler	1.11	0.00214	4.67	4.5
2nd-order Runge-Kutta	"	0.00461	2.17	4.0
4th-order Runge-Kutta	"	0.00570	1.75	6.2

(* The non-integral values appearing here were obtained from a curve of truncation error vs. increment size, and do not represent the actual number of increments used in computing the curve.)

The data above indicates that the 2nd-order Runge-Kutta method is significantly faster than either of the other methods for the ranges in distance and in truncation error considered. An unexpected result is that for errors on the order of one percent, the 4th-order Runge-Kutta method is slower than the Euler method. As the error decreases, both higher order methods become increasingly superior to the Euler method. Though it is clearly understood that the above results apply to the solution of a particular set of differential equations, for a given set of initial conditions, and for a particular interval, they nevertheless illustrate the importance of considering higher order methods of calculation and, further, of providing alternate methods, when planning a program of numerical analysis.

It is planned to continue these studies of truncation error in intervals successively further downstream. This will be done on a limited scale of effort while continuing Aerothermopressor performance calculations. The latter will be carried out using what is considered to be a conservative increment size.

The Aerothermopressor development program is being carried out at M.I.T. under the sponsorship of the Office of Naval Research and is directed by Professor Ascher H. Shapiro of the Department of Mechanical Engineering. The theoretical aspects of the problem treated by Whirlwind I are being carried out by Dr. Bruce D. Gavril.

B.D.Gavril
Mechanical Engineering

122 N. COULOMB WAVE FUNCTIONS

See Section 2.2 of Part I.

123 B,N. EARTH RESISTIVITY INTERPRETATION

See Section 2.2 of Part I.

126 D. DATA REDUCTION

Problem 126 is a very large data-reduction program for use in the Servomechanisms Laboratory. The overall problem is composed of many component sections which have been developed separately and are now being combined into complete prototype programs. Descriptions of the various component sections have appeared in past quarterly reports. After the development and testing of the prototype Whirlwind programs are completed, the programs will be re-coded for other, commercially available, large scale computers, (probably the ERA 1103, IBM 701 and IBM 704 computers),for use by interested agencies for actual data reduction at other locations. The programs are currently being developed by Douglas T. Ross and David F. McAvinn with the assistance of Miss Dorothy A. Hamilton, Servomechanisms Laboratory staff members. This work is sponsored by the Air Force Armament Laboratory through DIC Project 7138.

The nature of the problem requires not only extreme automaticity and efficiency in the actual running of the program, but also the presence of human operators in the computation loop for the purpose of decision making and program modification. For this reason extensive use is made of output oscilloscopes so that the computer can communicate with the human, and manual intervention registers so that the human can communicate with the computer in terms of broad ideas, while the computer is running, and have the computer program translate these ideas into the detailed steps necessary for program modification to conform to the human operator's decision. The program which does this translation and modification is called the Manual Intervention Program (MIV). The most recent version of the prototype data-reduction program is called the Basic Evaluation Program.

On June 1 and 2, 1955 a Data Reduction Symposium was held at the Barta Building under the sponsorship of the Servomechanisms Laboratory. The program included detailed considerations of hardware and programming for manual intervention switch inputs and scope-type outputs as well as the use of these devices for incorporating the human operator into the automatic computation loop both for routine computer operation and for large scale data reduction. Talks were presented by personnel of the Lincoln, Digital Computer and Servomechanisms Laboratories. Demonstrations included the operation of the Comprehensive System Utility Routines, the programs of Problem 126 and a special Guided Missile Launch Simulator program written under Problem 126 to demonstrate the use of the Charactron tube on the Memory Test Computer at Bedford. A tour of the Charactron and Typotron manufacturing facilities at Barta Building completed the program

The Basic Evaluation program has been rewritten to eliminate the use of buffers and to include an additional set of equations. Some progress has been made in the rewriting of the Manual Intervention Program so that it can use an arbitrary number of drum groups and have facilities for easy expansion.

The so-called Part I Program which has been in use for over a year is being rewritten for more flexibility and speed. In the process a new (24,6) square root routine has been devised which uses a combination of Whirlwind operations and direct modification and entry into the Programmed Arithmetic routines to obtain a square root in 5 milliseconds instead of the 31 milliseconds required for the fastest routine in the Subroutine Library.

A Basic Input-Translation Program for the ERA 1103 Computer is being written in 1103 code for translation by the program of Problem 256. The routine allows the use of mnemonic code, absolute addresses, and integers to any base, and includes many checks for illegal characters and combinations. It follows the conventions of Problem 256 and is intended to be used for making corrections to 1103 programs while at the site of the 1103 computer.

D.T.Ross
Servomechanisms Lab

131. SPECIAL PROBLEMS (STAFF TRAINING, DEMONSTRATIONS, ETC.)

As part of the S and EC Group activity, a two-week CS Training Course is offered when necessary to new users of WWI. In the past, this course has consisted solely of lectures and discussion with no opportunity for actual use of the computer.

In an attempt to increase the effectiveness of the course, WWI time was made available to students when the course was given during this quarterly period. The students coded a change-making problem, which was chosen to be simple enough for even novice programmers to complete in a short time. About twelve of the enrolled students ran programs during the time allotted for this purpose.

During the past three months, nine groups visited the Laboratory. The affiliations of some of the larger groups are given in Appendix 3.

132 D. SUBROUTINES FOR THE NUMERICALLY CONTROLLED MILLING MACHINE

During this period, an Electrical Engineer's thesis entitled Automatic Data Preparation for Numerically Controlled Machine Tools was submitted by J.H.Runyon to the MIT Electrical Engineering Department. This report contains chapters on metal-cutting geometry, numerical methods, description of WWI subroutines written especially for the milling machine, description of milling machine tape-preparation routines, results of a study of computing facilities outside MIT, and suggestions for future extensions of the present study. An appendix contains codes of the library subroutines used during the study and detailed descriptions of their operation. Portions of this thesis will be available in engineering report form at a later data.

Application and further development of the subroutine library were continued. Two subroutines were successfully tested. One is for more accurate feedrate control than was possible with the feedrate-control subroutine previously written and tested. The other subroutine is for computing cutter-center offsets given two orthogonal tangents to the surface at the point under consideration. Milling machine tape was prepared for rough and finish cuts on a cam for Stromberg-Carlson Corporation. Another milling machine tape was prepared for a spiral to be used in a demonstration of a new numerically controlled spin mill at Giddings and Lewis Corporation in Fond du Lac, Wisconsin.

The programmers for this problem were J.H.Runyon and T. Nagle of the Servomechanisms Laboratory, MIT.

J.H.Runyon
Servomechanisms Laboratory

141. S AND EC SUBROUTINE STUDY

An error was found in library subroutine LSR FU 4 b. This subroutine was designed to find sines and cosines of large angles, reducing the angles to first quadrant equivalents by means of non-interpreted instructions, thereby shortening the calculation time. However, this reduction was found to be in error in certain cases. The subroutine has been corrected and is now being tested.

A seven-point Gauss-integration subroutine has been coded and tested.

Two routines for the direct or delayed print-out of (30,0) and (15,0) decimal fractions, available in an older subroutine library, have been brought up to date and are now available.

LSR OS 2, Decimal integer scope output routine, has been rewritten to conform to the present status of scope decoders.

144 N. SELF-CONSISTENT MOLECULAR ORBITAL

This project has been described in previous reports by Dr. A. Meckler, who has completed the revisions which he undertook shortly before leaving the M.I.T. Solid State and Molecular Theory Group. (See Summary Report No. 40, p. 17). A second revision has been completed by Dr. R. Nesbet and tested on simple examples. The program is now designed to carry out approximate Hartree-Fock calculations for wave-functions of arbitrary configuration, using the method of symmetry and equivalence restrictions. In the present program, all one-electron integrals are transformed to the orthonormal basis of self-consistent orbitals after the last iteration. The Schmidt orthonormalization process is used instead of the earlier $\Delta^{-1/2}$ technique. Convergence has been made more rapid by an extrapolation

method. The program is being tested in a series of calculations of gradually increasing complexity, described under Problem 288.

R. K. Nesbet
Solid State and
Molecular Theory
Group

155 N. SYNOPTIC CLIMATOLOGY

During the last quarterly period, the objective of the project has been to specify and predict 5 Day Mean Anomalies for both temperature and precipitation using the same statistical methods which the project has been using for the past two years. This is a continuation of work which has been in progress for the past few months. Because of the amount of data used, and the size of the matrices involved, it became necessary to program the arithmetic operations; several programs have been written for this purpose.

At the present time this particular phase of the problem is nearing completion. Further comments concerning this problem cannot be made until all results have been computed and analyzed.

Programming is being performed by Miss Elizabeth Kelley under the supervision of Professor Henry G. Houghton of the M.I.T. Meteorology Department.

E. A. Kelley
Meteorology

156 L. EVALUATION OF THE REFLECTION COEFFICIENT IN A SEMI-INFINITE RECTANGULAR WAVE GUIDE

Previous results for the range $0 \leq \alpha < \pi^2$ indicated that this section of the problem should be recoded using Simpson's Rule instead of the Trapezoidal Rule. It was then decided to use Simpson's Rule for the other remaining sections of the problem as well, i.e., for the parts of the problem in the range $-30 \leq \alpha < 0$. Preliminary codes were written and run for these two latter sections, yielding satisfactory results. These preliminary codes are to be converted to final codes, a relatively minor task, and then run.

A. Balser

172 B,N. OVERLAP INTEGRALS OF MOLECULAR AND CRYSTAL PHYSICS

See Section 2.2 of Part I.

193 L. EIGENVALUE PROBLEM FOR PROPAGATION OF ELECTROMAGNETIC WAVES

This problem has been described in detail in Summary Report No. 39. It arose at Lincoln Laboratory in connection with the problem of calculating the electromagnetic radio frequency field radiated by a Hertzian dipole to points well beyond the horizon over a perfectly reflecting earth through the lower atmosphere idealized to be an inhomogeneous medium with index of refraction decreasing linearly with height.

Numerical computations were continued during the past quarter.

H. B. Dwight
Lincoln Laboratory

194 B,N AN AUGMENTED PLANE WAVE METHOD AS APPLIED TO SODIUM

An attempt has been made to keep input to its strictest minimum in a program which calculates certain electron energies in face-centered and body-centered crystals.

The program as it now stands makes much use of punchouts. In the first stage the input consists of the reduced wave vector (specified as integers) of the point in the Brillouin zone at which energies are to be calculated along with the lattice constant and the radius of the inscribed sphere of the unit crystal cell. The output consists of a punched tape and an oscilloscope display of the information punched. When to this tape is added certain other information, the tape contains all the physical constants necessary to characterize an augmented plane wave (APW) in ensuing calculations at the particular point in the Brillouin zone. This allows the input in all other parts of the calculation to be

integers. One can regard these integers, which are paired, as the two subscripts which characterize an APW. One subscript specifies the order of neighbor in reciprocal space to which the APW belongs and the other specifies the "band" to which it belongs. As a check, one subscript is always taken to be negative, the other always positive. It is then simple to program a check to see if a subscript has been missed.

In the next stage, parameters associated with the APW must be calculated. The input here is the initial tape along with a "subscript tape". The output is a punched tape of the calculated parameters followed by a scope display of these.

The third stage is an assembly stage where a certain subset of APW is to be assembled to form a subspace in which the Hamiltonian is to be diagonalized. The first part of the input consists of all the tapes from the previous stage which contain the component APW of the subspace desired. These tapes are read into the computer while the program checks to see if they refer to the APW at the point required. This feature guards against tape mixups. Then a "subscript" tape is fed in and completes the input. As another safeguard, the program checks to see if all the component APW asked for have been read in. In this "subscript" tape the order of the subscripts are important because the secular equation routine first solves the secular equation with one APW, then two, then three, etc., until the subspace is exhausted. The output of this stage is a punched tape which now characterizes a subspace of APW at a point in reciprocal space. What remains to be specified is the particular symmetry the APW is to have.

This latter information is the input of the last stage: generation of matrix elements and diagonalization of the secular equation. The symmetry is specified by five integers. The first of these specifies the dimension of the representation to which the APW are to belong. The sign of this integer specifies the behavior under inversion. Three integers specify the basis of the representation. The first two of these integers specify the "projection" operator to be applied to the APW while a fourth integer specifies if the representation or its adjoint is to be given. If only the dimensionality is given the program itself computes the "projection" operator which leads to the fewest number of APW in the linear combination of APW which constitutes the symmetricized APW. Along with these five integers the tape from the previous stage completes the input. As output the secular equation (energy and overlap matrices) is punched out and displayed, and, of course, the eigenvalues and eigenvectors are displayed.

Much of the routine outlined above has been tested. In the meantime, calculations have been carried out at the points $(1,0,1)\pi/a, (0,0,0)\pi/a$, and $(2,0,0)\pi/a$ for one "band". These results indicate that for all but the symmetric states convergence even in one "band" is quite good. The convergence for the symmetric states, however, leads one to believe that other "bands" should be included. Further information can be found in the Quarterly Progress Reports of the Solid State and Molecular Theory Group.

M. M. Saffren
Solid State and
Molecular Theory Group

195 C. INTESTINAL MOTILITY

Problem 195 is a study of the effect of radiation upon the motility of the small intestine in the rabbit. The analysis of records is being performed using autocorrelation and Fourier transformation, both performed on WWI under the supervision of D. Hamilton of the MIT Servomechanisms Laboratory.

Analysis of a total of 89 motility records has been completed on WWI including photographic plotting of both autocorrelation and Fourier transform. Seven records are not yet completed.

Evaluation of analyzed records has just been started.

Dr. John Farrar
Evans Memorial
Hospital

199 N. LAMINAR BOUNDARY LAYER OF A STEADY, COMPRESSIBLE FLOW IN THE ENTRANCE REGION OF A TUBE

In connection with the research on heat-transfer coefficients for supersonic flow of air in a round tube, a theoretical investigation of the characteristics of the laminar

boundary layer in the entrance region has been carried out. The boundary layer equations of continuity, momentum, and energy are to be solved for specific entrance Mach numbers and thermal conditions at the tube wall.

Gill's method is used in the numerical integration of these equations.

A new program using CS for finding the correct initial conditions was run successfully for the solution of the first set of differential equations.

Another program is being prepared for the solution of the third set of differential equations.

T.Y.Toong
Mechanical Engineering

203 D,N. RESPONSE OF A FIVE STORY FRAME BUILDING UNDER DYNAMIC LOADING

See Section 2.2 of Part I.

204 N. EXCHANGE INTEGRALS BETWEEN REAL SLATER ORBITALS

Testing on this problem is being continued by P. Merryman of the Physics Department of the University of Chicago.

R.K.Nesbet
Solid State and
Molecular Theory Group

212 B,N. DISPERSION CURVES FOR SEISMIC WAVES: MULTILAYERED MEDIA

See Section 2.2 of Part I.

213 D. INDUSTRIAL PROCESS CONTROL STUDIES

These studies are being carried out by J.B.Reswick and T.P.Goodman of the MIT Mechanical Engineering Department under problem numbers 213 and 281.

The Machine Design Division of the Mechanical Engineering Department is engaged in a project to determine the characteristics of an industrial process from the random fluctuations in the input and output records during the normal course of operation of the process. The method used is to compute two statistical functions -- the autocorrelation of the input and the crosscorrelation between the input and output of the process. From these correlation functions, the characteristics of the process can be determined much more readily than from the original records (ref. 1); hence the investigation. These computations involve a large number of successive multiplications and additions, and hence can be carried out most readily on an automatic computer. In this investigation, correlations were performed on Whirlwind I, using programs developed at the MIT Servomechanisms Laboratory.

The first part of this investigation was reported in the Quarterly Report for the last quarter of 1954 and in reference 2.

The investigation has been continued in two directions:

(1) Operating records were obtained for a distillation column and a heat exchanger at the oil refinery of the Rock Island Refining Corporation, and correlation functions for these records were computed on WWI. Some preliminary results have been obtained on the characteristics of these processes (ref. 3), and some new electronic equipment is being designed in order to obtain additional information on process characteristics from the correlation functions.
(2) As part of a program to extend these methods to processes with multiple inputs (ref 3), a two-input process was simulated on an analogue computer and subjected to artificial random inputs. Correlation functions for the simulated process were computed on WWI.

It is planned to continue this investigation as additional operating records from industrial processes become available for analysis.

References

1. T. P. Goodman and J. B. Reswick, "Determination of System Characteristics from Normal Operating Records", ASME Paper No. 55-IRD-1, April, 1955.

2. C. M. Chang, "A New Technique of Determining System Characteristics from Normal Random Operating Records", Mech. Eng. Thesis, MIT, January, 1955.

3. T. P. Goodman, "Experimental Determination of System Characteristics from Correlation Measurements", Sc.D. Thesis, MIT, June, 1955.

J. B. Reswick
T. P. Goodman
Mechanical Engineering

217 N. VARIATION-PERTURBATION OF ATOMIC WAVE FUNCTION AND ENERGIES

See Section 2.2 of Part I.

218 N. TRANSFORMATION OF INTEGRALS FOR DIATOMIC MOLECULES

A program has been constructed which converts output information of Problem 234 into the form of input data required by the programs of Problem 144.

This program deals with sets of biquadratic linear functionals $[ij|k\ell]$ which are symmetric under interchange of indices i and j, of k and ℓ, or of the pairs (ij), $(k\ell)$. These functionals are actually integrals with certain additional symmetry properties which cause large blocks of them to vanish. The initial data are the blocks of independent non-vanishing integrals arising from a given set of basis functions. From these it is required to construct a tensor of the form

$$A^{k\ell}_{ij} = \sum_\sigma \left\{ C_0^\sigma [ij \mid k\ell]^\sigma + C_x^\sigma [ik \mid j\ell]^\sigma + C_x^\sigma [i\ell \mid jk]^\sigma \right\}$$

The indices are divided into a number of ranges, corresponding to basis functions of different symmetry types. Indices i and j must lie in the same range, which might be denoted by α, and k and ℓ in a single range β, not necessarily the same as α. When ranges α and β are the same they specify a single block of integrals $[\alpha\alpha \mid \alpha\alpha]$; otherwise, there are two blocks $[\alpha\alpha \mid \beta\beta]$ and $[\alpha\beta \mid \alpha\beta]$ from which integrals must be selected in computing $A^{k\ell}_{ij}$. In order to locate a given integral $[ij \mid k\ell]^\sigma$ on the auxiliary drum the indices must be permuted to a canonical order: $i \geq j$, $k \geq \ell$, and $(ij) \geq (k\ell)$, treated as two-digit numbers. The integrals of a given block occur in this order, which ensures that all independent integrals are included and that no equal integrals are repeated. If the index σ has more than one value, integrals $[ij \mid k\ell]^\sigma$ for the various values of σ follow each other on the auxiliary drum. The first address of each integral block is stored in a table in the core memory.

In the general case the coefficients C_0^σ and C_x^σ depend on both the values of α and β and their order, so $A^{k\ell}_{ij}$ is symmetric under interchange of indices i and j and of k and ℓ, but not of the pairs (ij), $(k\ell)$. For given α, i, and j $(i \geq j)$ all elements $A^{k\ell}_{ij}$ $(k \geq \ell)$ are to be planted in order on the auxiliary drum. The index β does not run through all ranges of indices and some may be repeated. However, index β runs through the same ranges in order for all values of α, and α runs through all ranges without repetition.

In calculations for which this program is to be used, single blocks $[ij \mid k\ell]^\sigma$ can be too long to be included in the core memory. Since elements must be picked out from arbitrary places in the block it appears to be impossible to avoid making drum transfers of single CS numbers (or sets of two or three when σ has several values) instead of the relatively more efficient block transfers. The tensor elements $A^{k\ell}_{ij}$ are transferred to the drum in blocks whenever a certain number have been calculated. Even though the program is forced to use single drum transfers, the over-all speed seems still to be limited primarily by the CS arithmetic and by the complicated WWI program needed to control the calculation and to compute drum addresses.

R. K. Nesbet
Solid State and
Molecular Theory
Group

224 N. COMPUTATIONS OF THE FIELDS OF VERTICAL VELOCITY AND HORIZONTAL DIVERGENCE

This problem determines the field of vertical air motion for a series of weather situations. A detailed description of the problem was given in Summary Report No. 41. The results will be analyzed by the Pressure Change Project under the supervision of Professor James M. Austin of the M.I.T. Meteorology Department.

The program is running successfully and results are being compiled. An unusual example of data processing, the program computes and displays about 15,000 five-digit words of useful information on 145 frames of film in about four and one-half minutes.

W. Wolf
Meteorology

225 B,N. NEUTRON-DEUTERON SCATTERING

See Section 2.2 of Part I.

226 D. INVESTIGATION OF THE VORTICITY FIELD IN THE GENERAL CIRCULATION OF THE ATMOSPHERE

Description of Problem

The physical processes which are important in the maintenance of the general circulation of the atmosphere are being investigated with the aid of a two parameter, non-linear, quasi-geostrophic model of atmospheric flow. The model makes use of the vorticity equation and the first law of thermodynamics and incorporates effects of nonadiabatic heating and friction as well as the vertical advection of vorticity and the transformation of horizontal vorticity into vertical vorticity. A spherical coordinate system with pressure as the vertical coordinate has been used in the derivation, and the model is being applied to the Northern Hemisphere from 15°N to 75°N latitude. The two parameters used to describe the flow are the 700 mb and 300 mb contour heights.

With the aid of the model described above it is planned to examine the role of various heating distributions in generating the gross features of the general circulation. In particular, solutions for adiabatic flow will be compared with those for:

a. a simple heating distribution derived from data on the mean monthly heat transports across latitude circles;

b. a heating distribution which takes into account the so-called "secondary" heat sources and sinks which arise because of differences between land and sea;

c. a succession of heating distributions of increasing complexity leading to a time dependent heating function which varies in the vertical as well as in the horizontal direction.

It is planned to iterate the solution for a period of several days starting with observed initial conditions. In addition, solutions will be obtained for the case in which the initial conditions are given by a fictitious flow pattern characterized by a random disturbance superimposed on a basic zonal current. These solutions will be iterated for an extended period and the day-to-day changes of the flow pattern studied in an attempt to gain some insight into the mechanism by which differential heating generates and maintains the observed features of the general circulation.

The equations of the model are of the following form.

(1) $$G(y)\,\nabla_s^2\frac{\partial h'}{\partial t} - H(y)\frac{\partial}{\partial y}\left(\frac{\partial h'}{\partial t}\right) - I(s_m, s_T; y)\frac{\partial h'}{\partial t} + N(h,h', s_m, s_T; \lambda, y) = 0$$

(2) $$\dot{P}_m = -(\text{const})\left[\frac{\partial h'}{\partial t} + J_s(h,h') + \text{const}\,\bar{\zeta}\right]$$

(3) $$\frac{\partial s_m}{\partial t} + F(h,h',s_m,s_T,\dot{P}_m;\lambda,y) = 0$$

(4) $$G(y)\nabla_s^2 h - H(y)\frac{\partial h}{\partial y} = s_m$$

(5) $$s_T = G(y)\nabla_s^2 h' - H(y)\frac{\partial h'}{\partial y}$$

In these equations λ, y, and t are the space and time coordinates, respectively, F(), G(), H(), I(), $\bar{\zeta}$, and N() are known functions of the initial conditions, and,

h = geopotential height of a pressure surface

h' = geopotential thickness between two pressure surfaces

s_m = vorticity at the mean pressure level

s_T = thermal vorticity

$\dot{P}_m$ = vertical vorticity

$$\nabla_s^2() = F_1(y)\left[\frac{\partial^2()}{\partial\lambda^2} + \frac{\partial^2()}{\partial y^2}\right]$$

$$J_s(\psi,\phi) = F_1(y)\left(\frac{\partial\psi}{\partial\lambda}\frac{\partial\phi}{\partial y} - \frac{\partial\phi}{\partial\lambda}\frac{\partial\psi}{\partial y}\right)$$

The following is the procedure for solving the equations listed above:

1. Write the equations in finite difference form.
2. Initially, we are given the fields of h, h', s_m, s_T.
3. Solve equation (1) for $\frac{\partial h'}{\partial t}$ by relaxation.
4. Introduce $\frac{\partial h'}{\partial t}$ into equation (2) and evaluate $\dot{P}_m$.
5. Introduce $\dot{P}_m$ into equation (3) and evaluate $\frac{\partial s_m}{\partial t}$
6. Extrapolate $\frac{\partial h'}{\partial t}$ and $\frac{\partial s_m}{\partial t}$ over a short interval of time and add this value to the initial values of h' and s_m to obtain the values of h' and s_m at the new time.
7. Use these values of h' and s_m in equations (4) and (5) to obtain values of h (by relaxation) and s_T at the new time.
8. Having obtained the new fields of h, h', s_m and s_T, iterate the above procedure several times until the desired forecast is obtained.

Numerical Procedures

We had planned to solve the finite difference approximations to the equations of the model by relaxation, using a graded net of points over the hemisphere. However, we are now testing the feasibility of solving by an iterative application of the inverse matrices of the finite difference operators. This method of solution appears worthwhile in view of the relatively high speed of multiplication which Whirlwind I is capable of (approximately 45 microseconds). Furthermore, this method simplifies the solution for a graded net.

Progress and Future Plans

Programs for interpolating the original data to obtain values at the grid points of the graded net, and for computing the mean and thermal vorticity have been completed and successfully tested. Programs for computing the non-linear functions of λ and y have been written but not yet tested. A program for inverting a large order matrix (30th or 40th order) by partitioning and using library programs for matrix inversion and multiplication (15th to 20th order) has been written and is currently being tested.

Plans for the next quarter include completion of the matrix inversions, if this method is found to be feasible, and solution of the equations for at least one initial state.

Personnel

This research is being carried out under the sponsorship of the Air Force Cambridge Research Center by the following persons: R.L.Pfeffer, General Circulation Project, MIT; Duane Cooley, Geophysics Research Directorate; P. Castillo, General Circulation Project, MIT. Messrs. Cooley and Castillo are engaged in the programming.

R.L.Pfeffer
General Circulation Project

228 N. EVALUATION OF DIFFERENCE DIFFUSION EQUATION

See Section 2.2 of Part I.

230 C. DYNAMIC ANALYSIS OF BRIDGES

Saul Namyet of the MIT Department of Civil and Sanitary Engineering has obtained the final results from a long series of Whirlwind programs designed to determine the dynamic response of a single-degree-of-freedom system having a variety of resistance-displacement functions and subjected to a series of different loading functions.

The basic differential equation:

$$P_n - R_n = M\ddot{x}(t_n)$$

is evaluated by means of the second order difference equation:

$$(\Delta t)^2 \ddot{x}(t_n) = x(t_{n+1}) - 2x(t_n) + x(t_{n-1})$$

The results of this problem are contained in a project report on Contract No. AF 33(616)-2208 submitted to Wright Air Development Center, Wright-Patterson Air Force Base, Ohio.

S. Namyet
Civil and Sanitary
Engineering

235 B,N EIGENVALUES FOR A SPHEROIDAL SQUARE WELL

See Section 2.2 of Part I.

236 C. TRANSIENT RESPONSE OF AIRCRAFT STRUCTURES TO AERODYNAMIC HEATING

The transient response of aircraft structures to aerodynamic heating was initiated on January 3, 1955 by L.A.Schmit of the MIT Aeroelastic and Structures Research Laboratory. During the second quarter of 1955, work has continued on this problem. H. Parechanian has been responsible for the programming during this report period.

The over-all problem is that of investigating the influence of aerodynamic heating on the structural design of high-speed aircraft. One step in the solution of the over-all problem is to determine the transient temperature distributions in built-up aircraft structure. This phase requires the solution in generalized form of certain idealized heat flow problems. The second idealized heat flow problem (Problem II) has been formulated and solved. (See Summary Report No. 41 for a discussion of Problem I.)

Problem II can be briefly described as the thin plate and web problem. Heat enters the system by forced convection on the surface of the skin exposed to the external

flow (see Fig. 1). The contact joint which joins the skin and the web is assumed to have a heat transfer coefficient h_j and an effective joint contact length ℓ_j. The conductive heat flow is assumed to be essentially one-dimensional. The heat transfer coefficient is assumed constant and uniform over the exposed surface of the skin, and the adisbatic wall temperature (T_{aw}) is taken as a timewise step function. The temperature distribution is assumed to be uniform initially and the thermal properties of the skin and web materials are assumed constant.

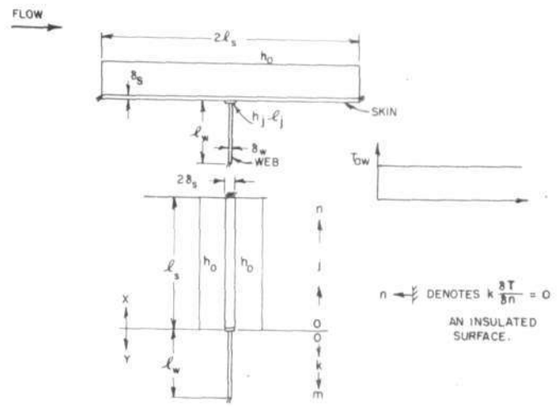

FIGURE I
SCHEMATIC REPRESENTATION OF PROBLEM II

The problem is formulated in terms of the following symbols:

T_{aw}	= adibatic wall temperature
h_o	= heat transfer coefficient (boundary layer to skin)
$2\ell_s$	= length of skin considered
ℓw	= length of web
δ_s	= skin thickness
δ_w	= web thickness
x	= location along skin
y	= location along web
t	= time
T	= temperature
ρ	= weight density

k = thermal conductivity

C_p = specific heat capacity

$\alpha = \frac{k}{\rho C_p}$ = thermal diffusivity

h_J = contact joint heat transfer coefficient

ℓ_J = effective joint contact length

Subscripts:

s refers to the skin or skin material

w refers to the web or web material

The heat balance equation for the skin is as follows:

(1) $$h_o(T_{aw} - T_s) + k_s \mathcal{J}_s \frac{\partial^2 T_s}{\partial x^2} = \rho_s C_{ps} \mathcal{J}_s \frac{\partial T_s}{\partial t}$$

The heat balance equation for the web is given by Eq. 2:

(2) $$k_w \mathcal{J}_w \frac{\partial^2 T_w}{\partial y^2} = \rho_w C_{pw} \mathcal{J}_w \frac{\partial T_w}{\partial t}$$

The initial condition is stated in Eq. 3:

(3) when $t=0$ $T_w = T_s = T_i$

The boundary conditions are formulated as follows:

(4) when $x=\ell_s$ $\frac{\partial T_s}{\partial x} = 0$

(5) when $y=\ell_w$ $\frac{\partial T_w}{\partial y} = 0$

(6) when $x=y=0$ $2\mathcal{J}_s k_s \frac{\partial T_s}{\partial x} = h_J \ell_J (T_s - T_w)$

(7) when $x=y=0$ $-\mathcal{J}_w k_w \frac{\partial T_w}{\partial y} = h_J \ell_J (T_x - T_w)$

The problem is put in nondimensional form by introducing the following additional notation:

$$\phi_s = \frac{T_{aw} - T_s}{T_{aw} - T_i} \quad ; \quad \phi_w = \frac{T_{aw} - T_w}{T_{aw} - T_i}$$

$$\bar{x} = \frac{x}{\ell_s} \quad ; \quad \bar{y} = \frac{y}{\ell_s}$$

$$\bar{t} = \frac{k_s}{\rho_s C_{ps} \ell_s^2} t \quad ; \quad \beta_s = \frac{k_s \mathcal{J}_s}{h_o \ell_s^2}$$

$$P = \frac{h_J \ell_J \ell_s}{2 \mathcal{J}_s k_s} \quad ; \quad Q = \frac{h_J \ell_J \ell_w}{\mathcal{J}_w k_w} \quad ; \lambda = \frac{\alpha_s}{\alpha_w} \left(\frac{\ell_w}{\ell_s}\right)^2$$

With the notation above, the problem defined by Eq. 1 through Eq. 7 can be stated in nondimensional form as a four parameter problem.

(1a) $$\frac{\partial^2 \phi_s}{\partial \bar{x}^2} = \frac{\partial \phi_s}{\partial \bar{t}} = \frac{1}{\beta_s} \phi_s$$

(2a) $$\frac{\partial^2 \phi_w}{\partial \bar{y}^2} = \frac{\partial \phi_w}{\partial \bar{t}} \lambda$$

(3a) when $\bar{t} = 0$ $\phi_s = \phi_w = 1$

(4a) when $\bar{x} = 1$ $\frac{\partial \phi_s}{\partial \bar{x}} = 0$

(5a) when $\bar{y} = 1$ $\frac{\partial \phi_w}{\partial \bar{y}} = 0$

(6a) when $\bar{x} = \bar{y} = 0$ $\frac{\partial \phi_s}{\partial \bar{x}} = P\left[\phi_s(\bar{t}, 0) - \phi_w(\bar{t}, 0)\right]$

(7a) when $\bar{x} = \bar{y} = 0$ $\frac{\partial \phi_w}{\partial \bar{y}} = Q\left[\phi_w(\bar{t}, 0) - \phi_s(\bar{t}, 0)\right]$

Consider the skin to be divided into n geometric elements of length $\Delta\bar{x} = \frac{1}{n}$ where it is understood that j refers to the jth skin element. Consider the web to be divided into m geometric elements of length $\Delta\bar{y} = \frac{1}{m}$ where it is understood that k refers to the kth web element. Let i refer to the ith time increment. If the second difference approximation is used for the first derivatives $\frac{\partial \phi_s}{\partial \bar{x}}$ and $\frac{\partial \phi_w}{\partial \bar{y}}$ at $\bar{x} = \bar{y} = 0$, while the first difference approximation is used elsewhere, the uncoupled forward finite difference formulation can be summarized by Eq. 8 through Eq. 13.

Let $N = \frac{\Delta\bar{t}}{(\Delta\bar{x})^2}$ and $M = \frac{\Delta\bar{t}}{(\Delta\bar{y})^2}$.

when $j = n$

(8) $$\phi_s(i+1,n) = \left[1 - \frac{\Delta\bar{t}}{\beta_s} - N\right] \phi_s(i,n) + N\phi_s(i,n-1)$$

when $1 \leq j \leq n-1$

(9) $$\phi_s(i+1,j) = N\,\phi_s(i,j-1) + \left[1 - \frac{\Delta\bar{t}}{\beta_s} - 2N\right] \phi_s(i,j) + N\,\phi_s(i,j+1)$$

when $j = 0$

(10) $$\phi_s(i+1,0) = \frac{1}{9+6P\Delta\bar{x}+6Q\Delta\bar{y}} \left[(8Q\Delta\bar{y}+12)\,\phi_s(i+1,1) - (3+2Q\Delta\bar{y})\right.$$
$$\left.\phi_s(i+1,2) + 8P\Delta\bar{x}\;\phi_w(i+1,1) - 2P\Delta\bar{x}\;\phi_w(i+1,2)\right]$$

when $k = 0$

(11) $$\phi_w(i+1,0) = \frac{1}{9+6P\Delta\bar{x}+6Q\Delta\bar{y}} \left[(8P\Delta\bar{x}+12)\,\phi_w(i+1,1) - (3+2P\Delta\bar{x})\right.$$
$$\left.\phi_w(i+1,2) + 8Q\Delta\bar{y}\;\phi_s(i+1,1) - 2Q\Delta\bar{y}\;\phi_s(i+1,2)\right]$$

when $1 \leq k \leq m-1$

$$\phi_w(i+1,k) = \frac{M}{\lambda}\phi_w(i,k-1) + \left[1 - \frac{2M}{\lambda}\right]\phi_w(i,k) + \frac{M}{\lambda}\phi_w(i,k+1) \tag{12}$$

when $k = m$

$$\phi_w(i+1,m) = \frac{M}{\lambda}\phi_w(i,m-1) + \left[1 - \frac{M}{\lambda}\right]\phi_w(i,m) \tag{13}$$

Once $\Delta\bar{x}$ and $\Delta\bar{y}$ are assigned, the selection of $\Delta\bar{t}$ in order to prevent divergent oscillation of the difference solution is a routine matter. (See Reference 1.) For the finite difference equations to be stable the increments selected for $\Delta\bar{x}$, $\Delta\bar{y}$, and $\Delta\bar{t}$ must be such that the following criteria are satisfied:

$$\frac{(\Delta\bar{x})^2}{\Delta\bar{t}} \geq \frac{2}{1 - \frac{\Delta\bar{t}}{2\beta_s}} \tag{14}$$

$$\frac{(\Delta\bar{y})^2}{\Delta\bar{t}} \geq \frac{2}{\lambda} \tag{15}$$

Satisfactory damping of convergent oscillations has been obtained by trial.

The final production program is based on a thirty element physical grid (n=m=15). Given the numerical values of the four parameters β_s, P, Θ and λ as well as a value of $\Delta\bar{t}$ the program computes $\{\phi_i\}$ from $\{\phi_{i-1}\}$. At the end of each time cycle the complete nondimensional temperature distribution $\{\phi_i\}$ for nondimensional time $\bar{t} = i\Delta\bar{t}$ is available in high-speed storage. Whenever $(1-\phi_s)$ at $j = 0$ or $(1-\phi_w)$ at $k = 0$ reaches 0.1, 0.2,...,etc., up to 0.9 at intervals of 0.1 the nondimensional temperature distribution ϕ_i at that time is stored on the magnetic drum. At the end of the computing phase for one case there are eighteen nondimensional temperature distributions, the nondimensional times associated with each distribution, and the numerical values at the given parameters β_s, P, Θ, λ and $\Delta\bar{t}$, stored on the magnetic drum. It is possible, with the present program, to compute and store the results for as many as ten cases before introducing the output display tapes. The efficiency of the computing phase of this program is good because the basic temperature distribution cycle, which constitutes a major portion of the computation, is carried out in WWI rather than CS II.

The first output tape yields a total of seven scope frames per case. The first four frames plot $(1-\phi)$ versus $\bar{x}$ and $\bar{y}$ for each of eighteen values of $\bar{t}$. The fifth frame is a plot of $(1-\phi_s)$ versus $\bar{t}$ for $j = 0, 1, 2$ etc., up to 15. The sixth frame is a plot of $(1-\phi_w)$ versus t for $k = 0, 1, 2$, etc., up to 15. The seventh frame is an alphanumerical scope display of the given quantities which define a case (β_s, P, Θ, λ, and $\Delta\bar{t}$), the eighteen pertinent times for which temperature distributions are available, and the final values of $\{\phi_i\}$. The final values of $\{\phi_i\}$ would serve as initial condition in the event that it ever became necessary to carry the calculation nearer to the steady state condition.

The second output (fp) tape displays all the information stored on the magnetic drum. This information is displayed on the scope in decimal fraction form. Since all the values of ϕ are between zero and unity the display gives all the values of ϕ to four decimal places in numerical, and immediately usable, form. It should be noted that for some engineering applications the graphical displays provided by the first output tape would be sufficiently accurate.

Work on Problem II is essentially complete. During the next report period, work will continue on the over-all problem. The computation of the transient thermal stresses which result from the temperature gradients will be considered.

Reference

1. Hildebrand, F.B., Methods of Applied Mathematics, Prentice Hall, Inc., New York, 1952, p. 323-345.

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238 B,N. SELF-CONSISTENT CALCULATIONS OF NUCLEAR MASS DENSITY

See Section 2.2 of Part I.

239 C. GUIDANCE AND CONTROL

This problem was described in the previous quarterly report (Summary Report No. 41). After several test runs, the CS II program ran successfully and four runs were made. A "George" coded program (that is, a routine coded in the algebraic system described in previous reports under Problem 108) has now been written for this problem but not tested.

J.H.Laning, Jr.
Instrumentation
Laboratory

241 B,N. TRANSIENTS IN DISTILLATION COLUMNS

The study of an ideal model of a fractionation tower which is undergoing changes in its operating conditions with time has been continued. A program has been written which can be used to calculate the plate compositions of a column in which the feed composition has undergone a step change but the product compositions are maintained constant by controlling the liquid-vapor ratios in the upper and lower parts of the column. Predicted values of liquid-vapor ratios from instantaneous compositions on plates between the feed plate and the top plate are also calculated as though the column were operating at equilibrium. Similarly predicted values of liquid-vapor ratios in the lower part of the column are calculated from instantaneous compositions of plates between the feed plate and the bottom plate.

From these data it is hoped to obtain correlations that will indicate: (1) the simplest method for controlling a column by introducing a delay factor when using a single intermediary plate composition in controlling the reflux ratio in the upper part of the column or the heat load to the reboiler; (2) more exact control of a column by using (a) more than one plate composition in each part of the column, (b) the time derivative of the composition together with its instantaneous value, or (c) the instantaneous plate composition together with the composition of the plate at some earlier time.

S.H.Davis, Jr.
Chemical Engineering

242 N. NUMBER OF STRUCTURES OF RELATIONS ON FINITE SET

See Section 2.2 of Part I.

245 N. THEORY OF NEUTRON REACTIONS

In the study of neutron reactions described in Summary Report No. 41, two programs, one for finding the power series solution to start the solution of the differential equation and the other for the solution itself and the cross sections have been written and tested separately. They have been combined into a master program which for any given x will find the cross sections for any range of X_o^2 by the use of a suitable parameter tape. The program has been tested satisfactorily for known values of the cross sections. Trouble of unknown origin arose in the first major run but as soon as this is cleared up it is planned to run the program for $\ell = 2$, $\xi = .15$ finding the cross sections for x = .4(.4) 4.4 and $X_o^2 =$ 0(5) 160 for each X_o^2, stopping when $X = \frac{X_o}{2.9}$.

The problem is being programmed for Professor H. Feshbach of the Physics Department by E. Campbell and E. Mack of the Joint Computing Group.

E. Campbell
Joint Computing Group

246 B,N. SCATTERING FROM OXYGEN

See Section 2.2 of Part I.

247 C. SURFACE PRESSURE PREDICTION

This problem has been carried out under the supervision of Professor J.G.Bryan of the MIT Mathematics Department. The problem, as described in Summary Report No. 41, evaluates the introduction of the quadratic component into the general linear scheme developed by Wadsworth and Malone for numerical forecasting.

The results will be included in a report to be submitted to the Geophysical Research Directorate of the U. S. Air Force.

250 C. TRANSLATION PROGRAM FOR THE NUMERICALLY CONTROLLED MILLING MACHINE

A preliminary version of the NCMM translation program has been completed. Tests of this version have shown that the transition from straight-line to circular cuts is, in certain cases, improperly computed by the routine. All other features described in Summary Report No. 41 are obtainable with the existing routine, and after this mistake is corrected, the system will be available in its entirety.

The vocabulary accepted by the translation program has been extended to include a "zero feed-rate" symbol. A zero feed-rate associated with a cutting instruction is defined to mean that the instruction is actually not to be executed, but that the cut preceding or following this instruction (as appropriate) is to be modified as if the instruction had been obeyed. Thus, the programmer may specify that a sequence of cuts is to begin as if the cutter had come from some point on the work or that it end as if the cutter were to go next to some other point. This notation is used to simplify the starting and the termination of a continuous sequence of cuts.

The existing preliminary version has been successfully used by Servomechanisms Laboratory personnel for programming a few pieces to be cut on the NCMM. Although the system has not yet been used sufficiently to permit a reliable statement of its effectiveness, some indication of its value has been obtained. The most difficult of the pieces that were tried requires about eight hours of hand computation. Programming the same piece for the translation routine required thirty-five minutes, to which must be added forty-seven seconds of Whirlwind I computer time for processing the problem. The other parts which were programmed indicate a similar reduction in programming time. All of the programs submitted for processing were error-free, despite the unfamiliar new notation.

The existing error in the preliminary version will be corrected, and the resulting routine will be subjected to test. The possibility of extending the system to more complicated cases, especially to three-dimensional problems, will be considered.

A. Siegel
Digital Computer
Laboratory

252 N. ANALYSIS OF TWO STORY STEEL FRAME BUILDING

See section 2.2 of Part I.

256 C. A WWI-ERA 1103 INPUT TRANSLATION PROGRAM

This two-pass input translation program was described in some detail in Summary Report No. 41. The program translates mnemonically coded programs for the ERA 1103 computer punched in Flexowriter form on paper tape into the standard bi-octal form directly acceptable by an 1103 computer. This program will be used by programmers working on Problem 126.

At the moment the program appears to be operating satisfactorily in all respects. However, automatic operation in the same manner as CS and other WWI coding systems will not be available until the new WWI input utility program (see Problem 100) is completed.

J. M. Frankovich
Digital Computer
Laboratory

257 C. HORIZONTAL STABILIZER ANALYSIS

The problem is to evaluate the deformations of the horizontal stabilizer of a typical present day fighter aircraft subjected to dynamic input conditions. Although the solution of the problem has been simplified by uncoupling the equations for rigid body motions of the aircraft and the equations for vibratory motions of the stabilizer, the rigid body response solutions serve as part of the input conditions to the vibratory equations of motion. Two separate programs have been set up, one for solution of the rigid body equations of motion and one for the vibratory equations of motion.

The rigid body motions considered are vertical translation and pitching rotation and, therefore, there are two rigid body equations. These equations are dependent nonlinear second-order differential equations; the nonlinearity arising in the aerodynamic force terms introduced by the dynamic input conditions. Because of the nonlinearity, conventional means cannot be used to solve these equations and therefore recourse to an approximate numerical scheme is necessary. The approximate numerical method employed is a numerical integration representation of each of the unknown variables and its derivatives in terms of previously evaluated values of the variable and its derivatives. The accuracy of a scheme of this nature (step-by-step numerical solution) is dependent on the increment of time employed in the analysis. The results obtained from this program for one input condition have been checked satisfactorily at various points by a desk computer solution of the same equations.

To solve for the vibratory motions of the horizontal stabilizer to dynamic input conditions, a dynamic model representation of the mass and stiffness distributions of the stabilizer was made. This representation consisted of seven lumped masses connected to one another by springs. Ordinarily the motions of this system could be represented by seven dependent linear differential equations which are solvable in closed form. For the particular structure and input conditions of the present problem, a small area of the structure incurs permanent buckles within a short time after initial application of the external forces. The properties of the spring which represents the stiffness distribution of the buckled area are altered from their initial pre-buckling values. As the buckles continue to increase, the properties of the spring continue to change, thereby making the equations of motion nonlinear in form and non-solvable by conventional closed form methods.

The nonlinear equations of the post-buckling region were linearized and then programmed for a step-by-step numerical solution on the Whirlwind Computer. The equations were linearized by dividing the post-buckling region into parts and making straight-line approximations in each of these parts. Although the individual sets of linearized equations for each part of the post-buckling region can be solved in closed form by Laplace Transformations, it is considerably more expedient to employ a step-by-step numerical solution on the Whirlwind Computer. The step-by-step numerical solution involves a numerical integration representation of each of the seven variables and its derivatives in terms of previously evaluated values of the variable and its derivatives.

The program operated satisfactorily for the seven lumped mass system described and for a particular set of input conditions. It is intended in the future to analyze a twelve lumped mass system subjected to various input conditions.

E. S. Criscione
Aeroelastic and
Structures Research
Laboratory

258 C. DYNAMIC ANALYSIS OF AN AIRCRAFT INTERCEPTOR.

This problem, described in Summary Report No. 41, has been completely checked out, and eight solutions have been run. The first three solutions were for the purpose of determining how well certain force and moment equations described the motion of an aircraft. These solutions were also used as check solutions for analogue computations performed on the M.I.T. Flight Simulator of the Dynamic Analysis and Control Laboratory.

As a result of the first three solutions and the analogue study, certain changes were indicated as desirable in the given equations and in some constants and input functions involved. These changes were applied to the Whirlwind programs, and new solutions were run to study the effect of the changes.

The results of the second series of runs are now being considered by engineers of the D.A.C. Laboratory and the Department of Aeronautical Engineering. Three

supplementary solutions are planned to complete the study.

K. Kavanagh
Dynamic Analysis
and Control
Laboratory

259 L. THE MEDIUM FREQUENCY IONOSPHERIC PROPAGATION STUDY

The earth's atmosphere between the altitudes of approximately 75 and 500 miles is partially ionized, and constitutes the region known as the ionosphere. Under certain circumstances and over certain frequency ranges, the ionosphere is capable of reflecting radio waves; this fact is the basis of most present-day long range communication and navigation systems. Also, most studies of the physical structure of the ionosphere utilize radio wave reflection as the principal experimental tool. For these reasons, the behavior of a radio wave that has undergone ionospheric reflection is of considerable interest.

The physical structure of the ionosphere appears to be quite complicated; it is neither homogeneous, nor isotropic, nor constant in time. It is subject to various periodic and aperiodic disturbances such as meteors, sunspots, and vagaries in the earth's magnetic field. No detailed physical theory of the ionosphere is known that satisfactorily accounts for all of the ionospheric phenomena that have been observed; the problem appears to be somewhat worse than giving a detailed theory of the troposphere (lower atmosphere) that would satisfactorily account for the weather.

However, certain types of ionospheric problems may prove amenable to a statistical type of treatment; it is a problem of this type that is the subject of the present study. When a steady-state, single-frequency radio wave is directed at the ionosphere, both the phase and amplitude of the returned wave are observed to vary in time (at a fixed point) and in space (at a fixed time). The statistical structure of this variability is of interest. For example, the probability distributions of amplitude and phase, the autocorrelation functions of amplitude and phase, the spatial correlation function of amplitude, the cross-correlation function of the amplitude at different points of space, and the correlation of amplitude fades and phase shifts are all important data.

In recent years, statistical theories of ionospheric reflection have been developed in which some of the statistical data above are predicted. Some of this theory is of a simplified nature (1) (2) (3), while some is based on highly refined physical theories (4) (5); however, the statistical results are often the same in either case (5). Some of the results predicted by this theory have been applied to ionospheric studies, and have been tested in highly limited ways (6) (7) (8). However, no thorough study of the (short-term) statistics of a reflected wave has yet been made, especially not under circumstances appropriate to communication and navigation systems. There exists considerable doubt as to the validity of the theories mentioned. The chief reason why no such study has been made in the past is the formidable amount of computation required; the determination of large numbers (several hundred) of correlation functions would be impossible, as a practical matter, in the absence of large-scale, high-speed computers.

The principal objective of the present study is to partially close this gap. From January through April, 1955, recordings of ionospherically reflected waves were made for five hours per day, in such a way that the statistical parameters mentioned above could be determined. (Under the circumstances of this experiment, about one hour is required for a statistical sample, so this is roughly equivalent to five independent samples per day.) The transmission path was from South Dartmouth, Mass., to Fort Belvoir, Virginia, a distance (great circle surface distance) of about 385 miles (620 Km.). The frequency employed was 543 kilocycles, and the hours of observation were from 1:00 AM to 6:00 AM (local time) daily. Under these circumstances, observed signals consist almost entirely of a "one-hop" wave reflected from what is known as the E region of the ionosphere.

The raw data obtained in the experiment have been transcribed onto punched paper tape for processing on Whirlwind I, where the statistical parameters will be computed. It is felt that the results obtained will be of interest both in basic ionosphere theory and in the practical design of communication and navigation systems.

This research was supported from January, 1951, through January, 1954, by the Department of State. Since January, 1954, it has been supported jointly by the U. S. Army, Navy, and Air Force. Both contracts have been with the Massachusetts Institute of Technology.

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260 N. ELECTRONIC ENERGY OF THE OH MOLECULE

Most of the work on this problem has so far been concerned with two major parts of the calculation, namely, the calculation of the many various integrals involved, and the evaluation of the "Lowdin Overlap Determinants" (LODS). (Ref. 1)

Calculation of Integrals

The basic set of one-particle functions are the Hartree-Fock 1s, 2s, and 2p atomic oxygen orbitals, and the hydrogen ground state function. From these, the Slater determinants (SDs) having the proper ground state symmetry of the OH molecule ($^2\pi$) are formed. A linear combination of these determinantal functions is then taken as the wave function describing the ground states of the molecule, and their coefficients determined by the variational principle to give the lowest ground state energy (secular equation). The elements of the secular equation are the one- and two-electron interaction integrals between the atomic orbitals. Using a program written for Whirlwind I by F. J. Corbató, many of the coulomb, exchange, hybrid, etc., one- and two-center integrals have been calculated so far. Up to several hundred radial integrations have been computed at one time (i.e., in one "run" of Whirlwind).

The two-center (one- and two-electron) integrals are calculated by first expanding the hydrogen function about the oxygen as center. For this purpose, Corbató, Karo, and Freeman have tested a program for calculating radial parts of the terms appearing in the expansion of the functions (ref. 2) $e^{-kr'}$ and $e^{-kr'}/r'$ about another center. The convergence of the terms in the integrals calculated this way seems good.

Lowdin Overlap Determinants

Basic to the use of non-orthogonal functions are the numerous overlap integrals which appear in the interaction of SDs.

A systematic way of handling the extraordinarily large number of terms that arise in this was recently given by Lowdin. As Lowdin has shown: the non-orthogonality integral of two Slater determinants is equal to the determinant of all the "non-orthogonality" integrals formed from the basic set of one-electron orbitals. There Overlap Determinants of Lowdin (LODs) as well as their minors (of first and second order)

provide a straightforward way of calculating the matrix elements of the Hamiltonian (or any other operator) between SDs made up from a non-orthogonal set of one-particle functions. Even so, the evaluation of the numerous minors and double minors is tedious even for our relatively simple case of 9 x 9 SDs. The simplifying features apparent in the use of orthogonal functions are missing, with the result that many integrals are not zero in our case. Even if an individual LOD is zero, its double minors are not, and the corresponding matrix elements of energy (consisting of two-electron integrals)give plentiful contributions to each term in the secular equation .

Lowdin's complete formalism is being used in our configurational interaction approach to the OH problem. Thus far the myriad of minors and double-minors arising from the 91 independent LODs formed from the thirteen basic SDs have been evaluated. It still remains, as a major task, to have them double checked.

This work will be used by A.J.Freeman in a PhD thesis in Solid State Physics.

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A.J.Freeman
Solid State and
Molecular Theory Group

261 C. FOURIER SYNTHESIS FOR CRYSTAL STRUCTURES

During the spring of 1955 several programs were set up for the use of Whirlwind I for crystal structure analysis as carried out in the Crystallographic Laboratory of the Department of Geology and Geophysics under the supervision of Professor M. J. Buerger.

The principal computational problems arising in crystal structure analysis can be described as follows:

1. Transformation of the experimentally found "data" (diffracted x-ray amplitudes) which are given in "reciprocal space" to the vector or electron density function in "real or crystal" space by means of a Fourier transformation according to the general formulas:

$$(1) \qquad P(xyz) = \sum_h \sum_k \sum_l F^2_{hkl} \cos 2\pi(hx + ky + lz)$$

and

$$(2) \qquad \rho(xyz) = \sum_h \sum_k \sum_l F_{hkl}\, e^{-2\pi i(hx + ky + lz)}$$

where P(xyz) is the three dimensional vector density or Patterson function, ρ (xyz) the three dimensional electron density function, F_{hkl} is the diffracted x-ray amplitude (in general a complex quantity), $F^2 = F \cdot F^*$ the diffracted x-ray intensity (always a real number), xyz are the coordinates in "real" space, and hkl the coordinates in "reciprocal" space.

2. The second problem is the reversed process, namely the transformation from "direct" to "reciprocal" space. This amounts to the computation of the scattered amplitude or structure factor F_{hkl} by means of a similar Fourier transform, according to the formula:

$$(3) \qquad F_{hkl} = \sum_j f_j e^{-2\pi i(hx_j + ky_j + lz_j)}$$

here f_j being the scattering power of the j^{th} atom, x_j, y_j, z_j the coordinates of the j^{th} atom and h, k, l the coordinates in "reciprocal" space.

For the use with Whirlwind,programs for special cases of equations (1) and (2) were prepared by S. M. Simpson, Jr., Assistant Professor in the Department of Geology and Geophysics and for equation (3) by G. Mahoney of the Whirlwind computer staff.

For both types the most general (noncentrosymmetrical and three dimensional) cases are in preparation.

These programs were applied by M. J. Buerger to the determination of the crystal structures of Wollastonite $CaSiO_3$ and Pectolite $CaNaSi_3O_8H$ and by Theodor Hahn to the computation of the three dimensional Patterson function of diglycinhydrochloride, from which it is hoped to obtain the solution of the structure by means of the "minimum function."

The investigations are being continued, and if successful, publication in a scientific journal is envisaged.

Prof. M. J. Buerger
Geology and
Geophysics

263 C. FLIGHT PATH OF AN AIRCRAFT DURING PULLUP

This problem was somewhat described in the Summary Report No. 41. It involves a set of 5 simultaneous first order differential equations plus a set of associated algebraic equations. The program for the problem was written for CS II using the Library of Subroutines for sine, cosine, square root, and differential equations.

The problem concerns high angle pull-up bombing where the flight path prior to pull-up is a straight-line dive at the target. A pull-up is then executed and calculations continue until a so-called release point occurs. The CS II problem solves the equations for each point (Δt = .1 sec) and considers each point a possible release point. A miss is computed for each point and by plotting misses against time the release points can be read off.

This is done for a variety of initial conditions and two sets of differential equations.

The programming for this problem was done by C. Block of the M.I.T. Instrumentation Laboratory.

C. Block
Instrumentation
Laboratory

264 C. OPTIMIZATION OF AIRCRAFT ALTERNATOR REGULATING SYSTEM

In the past, the problem of electrical machine design has been solved by some theory, many rules of thumb, and a copious amount of intuition and insight. The solution to the problem by this method may satisfy the design specifications, but the designer has no reason to expect his solution to be an optimum one. By optimum we mean in the sense of minimum weight, size, cost, or a combination of size, weight, and cost. The amount of calculation required to find such an optimum for a relatively intricate machine would be prohibitive if done by hand.

With the advent of the high-speed digital computer, the possibility exists of finding an optimum design for an electrical machine quickly and with economy. The techniques may be extended to optimize, not only the machine, but a system including a machine.

Two approaches toward the optimization have been proposed:

1. Trial and error: An electrical machine may be represented for digital computation as a program which determines quantities like heat rate, wave-form distortion, and short-circuit current from the dimensions and other physical parameters of the machine. The calculated quantities have constraints imposed on them by the design specifications. Using the trial and error approach, we would try many reasonable

combinations of dimensions and parameters, and select the one which satisfies the design specifications and gives the optimum machine (minimum weight, for example). This procedure can be improved by choosing the changes for the next trial on the basis of the results of previous trials - an educated trial and error approach.

2. As a minimization problem: The optimization problem, mathematically, is one of finding the minima of a function of m variables subject to n constraints. The variables are the dimensions and parameters of the machine, the constraints are the design specifications, and the function to be minimized is weight or size.

The first method has been used on a small scale using punched card techniques[1] with good results. Some work has been done by the writer on planning numerical procedures for the second method. These will be presented in a future report.

Progress in First Quarter

The first task that was undertaken was developing a sufficiently accurate calculation scheme for use with the computer over the ranges of the design parameters to be tested and to compare the results with the behavior of an actual machine. A 40-kva aircraft alternator is of particular interest to this project, and it was chosen as the machine to optimize.

The only special numerical procedure necessary here was a suitable representation of nonlinear functions, such as magnetization curves, for the computation. A third order interpolation routine was written which uses Gauss's forward formula.[2]

A program has been successfully run to check which design parameters are most important in matching each of the specifications.

Work is in progress to develop a more accurate calculation scheme for the alternator to be used with the optimization procedures. Plans call for the completion of the more accurate calculation scheme and tests of the optimization procedure by the end of the summer.

Personnel

R. M. Saunders - Associate Professor of Electrical Engineering (Visiting)

R. F. Nease - Research Assistant in Electrical Engineering

J. B. Dennis - Research Assistant in Electrical Engineering

The work reported here is being done at the Servomechanisms Laboratory under the sponsorship of the U. S. Air Force.

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J. B. Dennis
Servomechanisms
Laboratory

265 L. ELECTRON DIFFUSION IN AN ELECTROMAGNETIC FIELD

Solutions are desired for the second order boundary-value problem

$$\frac{1}{n}\frac{d^2\psi(y)}{dy^2} = (\epsilon\cos^2\pi y + g)\psi^3(y) - g\psi^2(y)$$

$$\left.\frac{d\psi}{dy}\right|_{y=.5} = \left.\frac{d\psi}{dy}\right|_{y=1.0} = 0$$

for values of the parameters ϵ, η, g.

A routine program was written which used an estimate of $\psi(.5)$ to get a solution to this initial value problem. This solution then was used to modify the estimate of $\psi(.5)$ by an amount depending on the degree by which $\left.\frac{d\psi}{dy}\right|_{y=1.0}$ differed from zero. A solution for $g = 2.0 \times 10^{-3}$, $\epsilon = 3.6 \times 10^{-3}$, $\eta = 5.6 \times 10^{-3}$ was determined. Changing η to 1.6×10^{5} caused the problem to be so sensitive to variation in $\psi(.5)$ that a variation of .005 in this value caused a variation of approximately 2×10^{19} in the value of $\psi(y)$ $.5 \leq y \leq 1.0$.

After trying several variations of this procedure, the technique of "feedback" was abandoned completely in favor of systematic trial and error using only the information that $\left.\frac{d\psi}{dy}\right|_{y=1.0}$ was positive or negative (with respect to a threshold interval about 0).

A subsequent solution has been obtained by this method.

D.N.Arden
Digital Computer
Laboratory

266 A. CALCULATIONS FOR THE MIT REACTOR

An investigation of the response of water-cooled reactors, with MTR type fuel elements, to slow changes in reactivity is under way.

A study will be made of the resulting time history of reactor power, fuel element temperature, and coolant channel pressure.

The system can be described by three interacting sets of equations: 1. the nuclear kinetics, 2. the thermodynamics, and 3. the fluid mechanics.

From the thermodynamics and fluid mechanics the average percentage of steam in the coolant channels is calculated as a function of the heat output of the reactor and the coolant flow rate.

Assuming fog flow, the properties of the steam-water mixture can be calculated and used in the Fanning equation.

(1) $$P_n = P_m + \frac{W^2}{gS^2}\left[(v_m - v_n) + \frac{\Delta L f_{mn} v_{mn}}{2r_h}\right] + \frac{\Delta L}{v_{mn}}$$

An energy balance between the entrance to the coolant channel and point n can be written

(2) $$C_p(T_n - T_o) + \frac{hZ_n}{W} = \frac{Q}{W} - \frac{W^2}{2S^2gJ}(v_n^2 - v_o^2) - \frac{L_n}{J}$$

These two equations, together with tabulated data, can be solved by trial and error for the pressure drop in the fuel element and the percent of steam.

For the nuclear kinetics the following equation is assumed:

(3) $$(\rho - \beta)\phi + \frac{1}{\nu\Sigma_{fission}}\sum_{1}^{1} \alpha_i C_i = \ell\frac{d\phi}{dt}$$

The reactivity can be written as

(4) $$\rho = \rho_e + \rho_m$$

in which ρ_e is the externally controlled reactivity and ρ_m changes with the amount of steam in the reactor.

The calculation of ρ_m is described below.

The critical mass of a critical reactor, or the period λ for non-critical reactor can be found by solving the equations:

(5) $$(\nabla \cdot D_s \nabla - \Sigma_s - \frac{\lambda}{r_s})\phi_s + p\,\Sigma_f\phi_f = 0$$

(6) $$\frac{k}{p}\Sigma_s\phi_s + (\nabla \cdot D_f \nabla - \Sigma_f - \frac{\lambda}{r_f})\phi_f = 0$$

The two-group model was assumed.

$\frac{\lambda}{r_f}$ was assumed = 0.

Only the highest eigenvalue solution of λ is considered to give $\phi = \phi_o e^{\lambda t}$.

For the calculation of the critical mass $\lambda = 0$ and the solution is obtained by varying the critical mass.

For the calculation of the period, the critical mass is constant and the solution is obtained by varying the period λ .

The solution is obtained by writing out the appropriate differential equations for the fuel and reflector regions and assuming the following conditions: 1.) the fluxes are continuous at the boundaries; 2.) the net currents are continuous at the boundaries; 3.) the flux is 0 at the outer boundary; 4.) spherical symmetry is assumed.

In this problem a four region reactor is calculated: non-multiplying region in the center, fuel in the next region and two non-multiplying regions on the outside.

In order to have a solvable set of equations, the determinant of the coefficients of the resulting 12 equations must equal zero.

The correct value of λ or the critical mass is found by trial and error.

In order to bypass difficulties in evaluating determinants with values close to zero, the following procedure was followed.

One of the arbitrary constants was assumed equal to one. Eleven of the twelve simultaneous equations were solved and the results substituted in the twelfth equation.

It was postulated that if the 12th equation were close to zero, all the other equations would be close to zero.

This turned out to be true in all cases calculated.

With the aid of perturbation theory it was possible to obtain expressions for the average thermal neutron lifetime, ℓ_m (Ref. 1) and the fractional change in K_∞ per unit fraction of steam produced in the fuel region, also called void coefficient (Ref. 1).

(7) $$\ell_m = \frac{\int_V \phi_s \phi_s^* \, dV}{\frac{k\,\Sigma_s r_s}{p}\int_V \phi_f^* \phi_s \, dV}$$

$$\frac{\frac{d(\frac{\Delta k}{k})}{d(V)_{H_2O}}}{V_{H_2O}} =$$

$$\frac{-p\Sigma_f \int_V \phi_s^* \phi_f dV + \Sigma_{(H_2O)s} \int_V \phi_s^* \phi_s dV + \Sigma_f \int_V \phi_f^* \phi_f dV - 3\Sigma_{s_{tr}} D_s^2 \int_V \nabla\phi_s^* \nabla\phi_s dV - 3\Sigma_{f_{tr}} D_f^2 \int_V \nabla\phi_f^* \nabla\phi_f dV}{\frac{k\,\Sigma_s}{p}\int_V \phi_f^* \phi_s dV}$$

These two quantities give insight into the behavior of a reactor in a transient. They will be calculated in each case studied. Knowing the pump characteristics, it will be possible to find for each power level the flow rate and the percent of steam. This in turn will give the change in reactivity calculated from perturbation theory.

Finally, after these values have been calculated and tabulated on WWI, a solution of equation (3) will be sought on an analogue computer.

The thermodynamics and hydraulic calculations were set up by R. Howard, Dynamic Analysis and Control Laboratory. The nuclear calculations setup and all programming for WWI were done by E. Troost. This program is being carried out for the Nuclear Reactor Project. No definite results have been obtained as yet.

Nomenclature

P	= pressure (lb/ft^2)
W	= total flow rate (lb/sec)
v	= specific volume (ft^3/lb)
L	= length (ft)
f	= fraction factor
ΔL	= $L_m - L_n$ (ft)
r_h	= hydraulic radius (ft)
g	= 32.2 ft. lbs. matter/sec.^{2} lbs.force
S	= area for flow (ft^2)
T	= temperature ($^\circ F$)
h	= heat of vaporization ($\frac{BTU}{lb}$)
Z_n	= steam flow rate (lbs/sec)
Q	= total heat added in section considered (BTU/sec)
J	= constant ($\frac{ft\text{-}lbs}{BTU}$)
C_p	= specific heat (BTU/lb $^\circ F$)

subscripts m and n refer to 2 different points along the length of the fuel element

subscript o refers to the entrance

ρ	= reactivity
β	= fraction of delayed neutrons
ν	= average number of neutrons per fission
$\Sigma_{fission}$	= macroscopic fission cross-section
α_1	= decay constant of i'th group of delayed neutron precursors
C_1	= concentration of i'th group of delayed neutron precursors
ℓ_m	= mean thermal neutron lifetime
t	= time (seconds)
∇	= the vector operator del. (or nabla)
D	= diffusion coefficient
ϕ	= neutron flux

Σ = macroscopic cross-section

k = infinite reproduction factor

p = resonance escape probability

r = average speed of neutrons

λ = period of the reactor

V = volume of the reactor

subscript s is for the slow group

f is for the fast group

tr is for transport cross-section

ϕ^* = indicates an adjoint flux

Reference

1. The formulas used were developed from perturbation theory by Dr. M. Benedict

M. Troost
Chemical Engineering

267 B. NUMERICALLY CONTROLLED MILLING MACHINE TURBINE BLADE

Machining warped surfaces on the NCMM involves the determination of a set of curves, each of which is to be approximated by a series of straight line segments. These curves are the intersections of the surfaces with a series of planes. The straight line segments used to approximate each curve lie in the plane whose intersection with the surface forms that curve. The path of the center of a cutting tool during the machinery operation is a series of straight lines between points on the normals to the surface and at a distance from the surface equal to the radius of a ball-shaped cutting tool.

The given data locates certain points on the surfaces of a turbine bucket for an aircraft jet engine currently in mass production. These points are given for the boundaries of eight cross sections on the airfoil portion of the bucket. At present, the problem is one of interpolation between given points on the cross sections and also between cross sections in order to define the surfaces in greater detail. The interpolation will result in a series of points representing curves formed by the intersections of the surfaces with planes parallel to the given cross sections.

A program to perform this interpolation has been written and is now being checked. It is based on the formula for polynomial interpolation in terms of divided differences

$$f(x) = y_o + \left[x_0x_1\right](x-x_0) + \left[x_0x_1x_2\right](x-x_0)(x-x_1) + \left[x_0x_1x_2x_3\right]$$

$$(x-x_0)(x-x_1)(x-x_2) + \ldots\ldots + \left[x_0x_1\ldots x_n\right](x-x_0)(x-x_1)\ldots(x-x_{n-1}).$$

Due to the error inherent in taking measurements of the given data from experimental models of airfoil sections, divided differences of higher than the third order show increasing divergence. The above formula was applied, therefore, to the third order divided differences. Work in the immediate future will consist of calculating the normals to the given surface at each point found in the above program, locating with reference to a set of orthogonal axes points on each normal at a distance from the surface equal to the radius of the cutting tool, and programming these points as the path of the tool center for the NCMM. At present, it is planned that this last program will be run on the NCMM and that the airfoil section of a pair of forging die blocks will actually be machined.

This project was begun with the idea of making a detailed economic evaluation of the conventional methods of machining the dies in question as compared to the method outlined above. Since this project is for academic credit toward a Bachelor's degree, time limitations have forced the elimination of further study into the economics of the two methods.

G. Bromfield
Business and
Engineering
Administration

268 C. EXTRAPOLATION TECHNIQUES

The problem under consideration was the extrapolation of certain time series arising from a particular, classified physical problem. Physical considerations made acceptable the hypothesis that the true series could be represented by means of low degree polynomials.

The following two methods of determining those polynomials were considered:

1. find the polynomial which is best in a weighted, least squares sense over a certain set of data points, or

2. first compute n+1 equally spaced and smoothed data points and then pass a polynomial of degree n through these points.

Whirlwind I was used to apply these methods to the particular data under consideration. From the results of these runs the accuracies of the two methods were compared in terms of the parameters of each method.

The second method proved to be superior for the data used. However, no general conclusions can be deduced from the study made.

S. A. Petrick
Servomechanisms
Laboratory

269 D. DYNAMIC BEHAVIOR OF SHEAR WALL TESTING MACHINE

See Section 2.2 of Part I.

270 B. CRITICAL MASS CALCULATIONS FOR CYLINDRICAL GEOMETRY

There are no exact analytic methods for calculating the critical masses of reflected reactors of more than one variable dimension. Spherically symmetric reactors can be calculated exactly, but cylindrical and parallelopiped ones cannot. One is forced either to a multigroup-multiregion point-by-point integration, or to finding some approximation to the exact solution. This problem will attempt to test approximations for cylindrical geometry.

Experimental critical masses of cylindrical reactors were obtained by A. H. Snell in 1946, for cores containing uranium 235, heavy water, and aluminum, surrounded by a heavy water reflector. If a satisfactory approximation were developed, it could be extended to the designs of other reactors, notably the projected MIT reactor.

The approximation now being tested is patterned after one developed by J. F. Hill. The exact analytic solutions are written for two cases: a radially reflected reactor and an end reflected one. Both solutions are obtained from the basic neutron diffusion equation, $\Delta^2\phi_{1,j} + B_1^2\phi_{1,j} = 0$. Two groups are used (fast and thermal) and two regions (core and reflector). The boundary conditions are that fluxes and neutron currents be continuous at the core-reflector interface, and that the fluxes vanish at the outer surface of the reflector.

Applying boundary conditions, the solutions are of the form (for the radially reflected case)

$AX + CY = FZ_1$ Fast Flux

$D_{1c}\left[AX' + CY'\right] = D_{1r}FZ_1'$ Fast Current

$S_1AX + S_2CY = S_3FZ_1 + GZ_2$ Slow Flux

$D_{1c}\left[S_1AX' + S_2CY'\right] = D_{1r}\left[S_3FZ_1' + GZ_2'\right]$ Slow Current

By Cramer's rule, the determinant of the coefficients, A, C, F, and G must equal zero for non-trivial solutions. Similar equations are found for the end reflected case except that X, Y, and Z are trigonometric and hyperbolic functions.

The solutions are then superimposed. One obtains (in Snell's case) a fourth and eighth order determinant which must simultaneously equal zero. All physical constants and dimensions are fixed, leaving two variables, critical mass and the radial-longitudinal buckling split, which correspond to the two determinants to be solved.

Progress to date has been the writing of the program, and the development of a subroutine to calculate the Bessel functions, J_0, J_1, I_0, I_1, K_0, and K_1. No critical mass calculation has yet been obtained.

An additional section has been written, but not tested, for calculation of the neutron lifetime and void coefficient. This is accomplished by taking a 100 x 100 mesh net covering the reactor, and integrating the fluxes numerically. First order perturbation theory is used.

This technique will also be useful for calculation of reactivity losses due to burnout poisoning, etc. In addition, plots of the radial and longitudinal fast and slow (real and adjoint) fluxes can be obtained.

If the method proves feasible, it will be extended to a four-region reactor, possibly with more energy groups.

Another approximation method exists, and it is planned to try it in the future. It involves expanding the fluxes in Fourier-sine and Fourier-Bessel series, and solving the resulting equations. It has the advantage of using three energy groups, and should be more accurate.

Nomenclature

D_{1c} = Fast core diffusion coefficient

D_{1r} = Fast reflector diffusion coefficient

D_{2c} = Slow core diffusion coefficient

D_{2r} = Slow reflector diffusion coefficient

R_c = Radius of core

R_r = Radius of reflector

S_1, S_2, S_3 = Coupling coefficients

$X = J_0(\mu_r R_c)$

$Y = I_0(\nu_r R_c)$

$$Z_1 = I_0(\xi_{1r} R_c) - \left[\frac{I_0(\xi_{1r} R_r)}{K_0(\xi_{1r} R_r)}\right] K_0(\xi_{1r} R_c)$$

$$Z_2 = I_0(\xi_{2r} R_c) - \left[\frac{I_0(\xi_{2r} R_r)}{K_0(\xi_{2r} R_r)}\right] K_0(\xi_{2r} R_c)$$

μ_r = Radial part of real buckling solution μ^2

ν_r = Radial part of imaginary buckling solution ν^2

ξ_{1r} = Analogue of reciprocal fast diffusion length

ξ_{2r} = Analogue of reciprocal slow diffusion length

$$\mu_r^2 + \mu_z^2 = \mu^2$$

$$\nu_r^2 + \nu_z^2 = \nu^2$$

$$\xi_{1r}^2 = \frac{1}{\tau} + \mu^2 - \mu_r^2$$

$$\xi_{2r}^2 = \frac{1}{L^2} + \mu^2 - \mu_r^2$$

τ = age in reflector

L^2 = thermal diffusion length in reflector

This study is being carried out in connection with an Sc. D. thesis for the Chemical Engineering Department.

J.R.Powell, Jr.
Chemical Engineering

271 B. EVALUATION OF A BEAM SPLITTING TECHNIQUE

This problem is a study of a proposed method of improving the accuracy with which conventional search radar systems determine target azimuth angles with respect to a fixed coordinate system. The operation of extracting azimuth information with an error less than the radar antenna's beam width is sometimes referred to as 'beam splitting'. The necessary programming details for WWI are being performed by Peter F. Engel, and the numerical results obtained will be incorporated into an M.S. thesis report to be submitted by him to the Department of Electrical Engineering at MIT in August, 1955. The problem represents one phase of a comparative analysis being conducted by Mr. Charlton M. Walter of the Applied Mathematics Section of the Computer Laboratory of the Air Force Cambridge Research Center. Mr. Robert Bernstein of the Electronics Research Laboratories at Columbia University was responsible for the application of a maximum likelihood estimation procedure to the beam splitting problem, and his work is described in detail in a report (Ref. 1) published by Columbia University.

The beam splitting problem is characterized, in part, by inherent statistical properties, and the particular solution under consideration here is essentially an application of the maximum likelihood estimation of a population parameter. A principal objective is to compute estimates of a target's azimuth position using simulated radar data, and to study the dispersion of these estimates about the known position.

The type of search radar system considered employs a continuously rotating antenna, radiating one or more directive beams of pulsed signals on an S-band microwave carrier. Pulse widths are in the vicinity of one tenth to four microseconds and are emitted at the common pulse repetition frequencies of 200 to 400 pulses per second. The radiation pattern of the antenna has the form $(\frac{\sin y}{y})^2$ where y is the angular deviation from the antenna axis.

As the radiated beam illuminates a target, reflected pulses are returned to the receiver over an arc length equal to the antenna's beam width. If there were no random noise or target scintillation present, the pulse amplitudes would follow the antenna pattern. In general, however, noise and scintillation combine with the echo signal and produce a skewed or distorted pattern from which it is difficult to determine the target's azimuth position by inspection. By considering each pulse in the azimuth scan as a single sample of a random variable whose probability distribution is known, the target azimuth, Θ, can be estimated.

A threshold, h, is set arbitrarily to quantize the individual pulses making up a complete scan into two discrete levels. The probability of a pulse being large enough to exceed the threshold level depends upon the gain of the antenna in the direction of the target at the instant the pulse was received. This in turn depends on the angle between the antenna axis and the azimuth of the target at that instant. The azimuth of the antenna's axis is always known, thus it is possible to formulate the probability, $f_1(x_1;\Theta,K)$, of receiving a pulse of amplitude x_1, as a function of target azimuth Θ, and the signal-to-noise ratio, K. If the simplifying assumption is made that successive pulses are statistically independent, a joint probability, $F(x_1,\ldots x_n;\Theta,K)$, for detecting all the pulses of

a scan can be formed. This distribution is called the likelihood function, L, for that particular scan,

$$(1) \qquad L = F(x_1 \cdots\cdots x_n \; ; \; \Theta, K) = \prod_1^n f_1(x_1 \; ; \; \Theta, K)$$

where n is the number of pulses per scan. The maximum likelihood method now consists in choosing as an estimate of the unknown population value of Θ, the particular value that renders L as great as possible. Since log L attains its maximum for the same value of Θ, as L, one has to solve the equation,

$$(2) \qquad \frac{\partial \log L}{\partial \Theta} = \sum_1^n \frac{\partial \log f_1}{\partial \Theta}(x_1 \; ; \; \Theta, K) = 0$$

The solution, $\hat{\Theta}$, is the desired target azimuth. Equation (2) can be reduced to a more convenient form,

$$(3) \qquad \sum_1^n W_1(k,\Theta)x_1 = 0$$

where $W_1(K,\Theta)$ is a weighting function of the two variables K and Θ. For computational purposes, W_1 can be plotted as a function of Θ, for discrete values of signal-to-noise ratio K.

After determining $\hat{\Theta}$ for each scan, the computer compares the answer with the known position of the target, and records the difference between the two. This is repeated for several video threshold levels, h, and for several values of n, to study the distributions of the dispersion in $\hat{\Theta}$.

Runs have been completed during which position estimates were computed at four discrete thresholds. In all four cases, 64 azimuth scans were processed, each of which contained 35 pulses. The resulting distributions of the estimates were found to have their mean values displaced from the true position by not more than 3 o/o of the antenna's beam width, and each distribution had a standard deviation about the mean of approximately 9 o/o of the beam width. The antenna's beam width is taken to be the distance between the 3 db points of the radiation pattern, and for the results cited above, was equal to one degree.

References

1. Technical Report T-1/128; Department of Electrical Engineering; Electronics Research Laboratories; Columbia University Engineering Center; 632 West 125th Street, New York 27, New York.

P. F. Engel
Electrical
Engineering

272 L. GENERAL RAYDIST SOLUTION

A system of equations has been derived by Dr. G. C. Sponsler of Lincoln Laboratory to provide for a particular set of data the position of an aircraft in latitude and longitude to an accuracy of better than six parts in one million.

The Raydist system employs one master radio receiver and three slave stations, any two of which may be used with the master station to provide data for a solution. A system of rectangular axes is referred to an origin located on a plane determined by the master and two slave stations. The aircraft is assumed to be on an ellipsoid. A system of three simultaneous quadratic equations is then derived, the coefficients of which are functions of Raydist data, and the solutions of which are rectangular coordinates of the aircraft. These rectangular coordinates are then transformed with latitude and longitude.

A program was written to solve the simultaneous system of equations by minimizing a sum of squares. It was learned, however, that convergence to the solution was too slow to render this method practical. Therefore, the system of equations was reduced to a single eighth degree polynomial equation by eliminating variables. A program for computing the

coefficients of this polynomial and obtaining its roots is now being written.

G. Mahoney
Digital Computer
Laboratory

273 N. ANALYSIS OF AIR SHOWER DATA

A group under the direction of Professor Bruno Rossi of the Physics Department of MIT is engaged in an experimental study of the size spectrum and arrival directions of large air showers. This group includes G. Clark, J. Earl, W. Kraushaar, J. Linsley, and F. Scherb. G. Clark and F. Scherb are primarily responsible for the design of the WWI analysis program.

The data for this study is obtained with twenty large scintillation counters arranged in an array 500 m. in diameter. The density of particles and the arrival time of the shower front at each of the twenty counters is recorded whenever an air shower strikes the array. From these data the size of the shower, the location of the core, and the direction of arrival are determined by digital computation.

The data consist of particle densities g_i (i = 1, 2, ...,20), relative arrival times t_i, the sidereal time, and various instrumental constants such as the counter locations x_i, y_i. The direction cosines ℓ, m, n of the shower axis relative to the ground are determined by finding those values of k, ℓ, and m which minimize the expression

$$\chi = \sum_{i=1}^{20} (k - \ell x_i - m y_i - c t_i)^2$$

n is related to ℓ and m by the equation

$$n = \sqrt{1 - \ell^2 - m^2}$$

The right ascension and declination of the shower axis are then computed from the direction cosines and the sidereal time.

The core location (X,Y) and shower size N are found by determining the values of α, β, X, and Y which minimize the expression

$$\psi = \sum_{i=1}^{20} (f_i - g_i)^2 w_i$$

where

$$f_i = \frac{\alpha e^{-\beta R_i}}{1 + R_i}$$

$$R_i = \sqrt{(X - x_i)^2 + (Y - y_i)^2 - \left[\ell(X - x_i) + m(Y - y_i)\right]^2}$$

and w_i is a weighting factor. The expression for f_i is a convenient empirical representation of the lateral density distribution of particles in an air shower. The size of the shower is then computed according to the equation

$$N = \int_C^\infty \frac{\alpha e^{-\beta R}}{1+R} \, 2\pi R \, dR$$

The first part of the computation program is devoted to the reduction of the experimental data to a form suitable for computation. The next part is a solution of the three first degree simultaneous equations for ℓ, m, and n (which come from the minimization requirement) and the computation of celestial coordinates. The last part of the program is the minimization of the expression ψ by means of iterative subroutine, and the calculation of N.

The program has been written and parts of it have been tested.

Effort will now be devoted to testing the program. When the program is successfully run, a thorough study will be made of the accuracy and resolution of the experimental and analysis setup using fictitious showers. Actual shower data will then be analyzed.

G. Clark
F. Scherb
Physics Department

274 N. MULTIPLE SCATTERING OF WAVES FROM A SPATIAL ARRAY OF SPHERICAL SCATTERERS

See Section 2.2 of Part I.

275 B. BUCKLING OF SHALLOW ELASTIC SHELLS

See Section 2.2 of Part I.

277 C. HORIZONTAL STABILIZER MODES, SHAPES AND FREQUENCIES

This problem involves the determination of natural mode shapes and frequencies of an airplane structure represented by a lumped mass dynamic model. The set of simultaneous linear equations which governs the free vibrations of the system is solved by a process of matrix iteration to yield the mode shapes and frequencies.

The set of simultaneous equations may be written in matrix form as:

$$[D]\{A\} = \frac{1}{w^2}\{A\}$$

The A's and w's are the modal coefficients and the frequencies respectively. The D matrix is computed by combining the deflection influence coefficients for the dynamic model, the constants pertaining to the mass and geometric properties of the aircraft structure, and the constants for the rigid body degrees of freedom of pitching and vertical translation.

The main tape for the program consists of a set-up for computing the D matrix, iterating for each mode shape and frequency, and a process for sweeping the D matrix to eliminate each successive mode after convergence. The tape has been prepared in a general form which limits neither the size of the D matrix nor the number of modes to be found. However, the size of the D matrix and the number of modes to be found are presently limited by the high-speed storage capacity of the computer.

A secondary tape, which is fed into the computer with the main tape, includes the matrix of influence coefficients, the constants associated with the two rigid body degrees of freedom, and a constant equal to the number of modes to be found. If it is so desired, it is a simple matter to eliminate either or both of the rigid body degrees of freedom and obtain cantilever mode shapes and frequencies.

Three problems have been solved during this period with satisfactory results. First a cantilevered beam model, consisting of three lumped masses, was run to determine the soundness of the program. Next, a cantilever model with seven masses was run and seven mode shapes and frequencies were obtained. Finally, a 12 x 12 matrix containing both pitching and vertical translation degrees of freedom successfully yielded the first five mode shapes and frequencies.

It is contemplated in the future to run investigations on various other models. It is also possible to use this program to solve other eigenvalue problems which arise in other branches of engineering.

N.P.Hobbs
K.R.Wetmore
Aeroelastic and
Structures Research
Laboratory

278 N. ENERGY LEVELS OF DIATOMIC HYDRIDES (LiH)

In a Quarterly Progress Report of the Solid State and Molecular Theory Group at MIT (Ref. 1) we considered briefly the problem of the electronic energy of the lithium hydride molecule. Using 1s and 2s atomic wave functions for the lithium atom, and a 1s

wave function for hydrogen, we found that six states occurred with proper ground state symmetry and proposed to examine the problem of interaction between these states as a function of the internuclear distance.

The specific atomic functions which we are using are the orthonormal 1s, 2s, and 2p Hartree-Fock wave functions for lithium (Ref. 2), and, located on the hydrogen atom, a normalized 1s Slater Atomic Orbital which is expanded about the lithium atom for purposes of calculation. This procedure of expanding an orbital located on one center about another center has been outlined by F.J.Corbató (Ref. 3) and is particularly simple for the analytic form we have chosen. The Hartree-Fock wave functions are, of course, orthogonal; but the hydrogen wave function has not been made orthogonal to the lithium wave functions so that the overlap integrals must be evaluated.

All of the one-electron and two-electron integrals have been obtained for the lithium atom taking into consideration the 1s, 2s, and 2p functions; and all of the additional overlap, one-electron, and two-electron integrals for the lithium hydride molecule near the observed internuclear distance, using only the 1s and 2s lithium functions and the hydrogen 1s function, have also been calculated. With the exception of the kinetic energy integrals the computations have been performed on the Whirlwind digital computer using the routines developed by F.J.Corbató (Ref. 3).

An intermediate calculation has been completed for the electronic energy of the neutral lithium atom as a partial check of our work. Using the 1s, 2s, and 2p Hartree-Fock lithium wave functions one may construct the possible determinantal wave functions for the ^2S and ^2P cases; from these, four states may be formed which possess the ^2S ground state symmetry and five states with ^2P symmetry. The single determinant representing the unexcited ^2S ground state gave an electronic energy within one-half per cent of the experimental value, in good agreement with that found by Fock and Petrashen (Ref. 4). When the matrix of interaction of the four ^2S states was diagonalized, there was an almost insignificant decrease of the electronic energy for the ground state. This seems to indicate that the configuration interaction with the excited states results in a negligible correction. The ^2P state was similarly but slightly lowered when configuration interaction with the four other excited states was included. The calculated value for the wave length of the transition between the ^2P and ^2S states was also within one-half per cent of that experimentally observed.

A preliminary valence bond calculation has been completed for the lithium hydride molecule near the observed internuclear distance. The value of the electronic binding energy for this single state was found to be about one-third of the observed value of 2.5 ± 0.2 electron volts given by a linear Birge-Sponer extrapolation (Ref. 5).

Attention at the moment is centered on combining the basic integrals which we have obtained, to form the Hamiltonian matrix and the overlap matrix. We shall be able then to determine the extent of configuration interaction in refining the valence bond calculation which has been made. We are also prepared to extend the treatment to a number of internuclear distances in the near future.

References

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F.J.Corbató, Quarterly Progress Report, Solid State and Molecular Theory Group, MIT, April 15, 1955, p. 44.

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5. A. G. Gaydon, Dissociation Energies and Spectra of Diatomic Molecules, Dover (1950) p. 210.

G.F.Koster
A.M.Karo
A.R.Olson
Solid State and
Molecular Theory
Group

280 B. CORRELATION FUNCTION

This problem concerns the application of the theory of Stationary Time Series to Meteorology. Specifically, it is concerned directly with the methods and theory of Linear Prediction as developed by Norbert Wiener which requires extensive use of harmonic analysis.

The work represents an attempt to extend the so-called factorization to more than two series and to set up the problem of determining the prediction operator for multiple series on a practical computational basis. So far as is known, no one has as yet obtained the prediction operator for two or more series by direct application of Wiener's theory.

The computational work can be separated as follows: obtaining correlation functions; obtaining spectra of these correlation functions and related functions; factorization (which leads directly to the prediction operator). At the present time, the first phase is essentially completed. It is expected that the entire problem will be completed during the next quarter.

The programming has been performed by R. E. Huschke, and B. Rankin is aiding in the theoretical considerations of the problem.

This research is being undertaken as a doctoral thesis in the Department of Meteorology, Massachusetts Institute of Technology.

P. Hanna
Meteorology

281 C. CORRELATIONS AND TRANSFORMS

See report under problem number 213 above.

282 B. HELICOPTER BLADE FLAPPING INSTABILITY

Equations describing the behaviour of a helicopter rotor blade having three degrees of freedom, flapping, bending, and torsion, were formulated. The analysis, which took full account of reverse flow effects, led to three differential equations each of which contained a term involving an integration over the span of the blade. These equations were solved by Gill's method, a step-by-step numerical integration procedure similar to the more familiar Runge-Kutta method. A program making use of this method was drawn up for use on Whirlwind I, Q6 II. The program will determine, for a particular flight condition, the transient response of the blade by evaluating and recording on the oscilloscope values of each of the degrees of freedom at fifteen degree intervals of the azimuth angle. It was found that the computer required approximately eight seconds to compute the values at each azimuth angle.

Runs were made to determine the effect on blade stability of a variation in each of the following: 1) reverse flow, 2) blade weight, 3) pitch-flap coupling angle, 4) rotor angular velocity, and 5) inclusion of a torsion degree of freedom.

The conclusions resulting from the above were: 1) inclusion of reverse flow effects lead to higher values of forward speed at which instability occurs than would otherwise be found, 2) at the flight speed investigated, the heavier the blade, the more stable it is, 3) on the basis of the runs made (only two in number), the pitch-flap coupling angle does not appreciably affect the damping of the flapping motion, and 4) due to lack of time, the author was not able to obtain any results from 4) and 5) above. However, initial results obtained while the "bugs" were being worked out of the tapes seem to indicate that the torsion degree of freedom has an important destabilizing effect.

A complete description of this problem, including all Whirlwind results, is presented in a Master's thesis submitted to the Department of Aeronautical Engineering.

P.J.Arcidiacono
Aeronautical Engineering

283 B. A STUDY OF ERROR-REDUCTION IN INFORMATION SYSTEMS

An attempt was made to simulate the error-reduction characteristics of a 15-node network by the calculation of several arbitrary measures of redundancy. Networks were chosen in which the measure of centrality as outlined by Bavelas was constant. The minimum number of steps to completion of a task was also kept constant. Connections between nodes were represented digitally as ones, no-connections as zeros. It was found

that networks which reduced zeros quickly (i.e., the rate of information transferred between nodes increased) had a high average redundancy and it was also found that networks which had horizontal connections (i.e., ties between members in a level) rather than vertical connections (ties between members in adjoining levels) exhibited an increasingly non-linear relation between redundancy and the number of steps toward completion of information transfer.

References

1. Christie, Lee S., "Organizations and Information Handling in Task Groups", JORSA, 2,2,1954.

2. Bavelas, Alex, "Communication Patterns in Task-Oriented Groups", Acoustical Society of America Journal, 22, 1950.

R.M.Oliver
Operations Research Group

285 N. AUGMENTED PLANE WAVE METHOD AS APPLIED TO CHROMIUM CRYSTAL

The radial Schroedinger equation integration routine has been modified to display wave functions numerically on the scope. This facilitates finding the range of energy for which the wave function remains essentially unchanged at a given radius. With this information, as has been pointed out by Leighton, the integration can be speeded up considerably.

Since all the routines described under problem 194 are used for this problem, some of those routines have been tested under this problem number.

M.M.Saffren
Solid State and Molecular Theory Group

286 B. RESPONSE OF THE HUMAN PILOT IN A DAY SUPERIORITY TYPE FIGHTER FLYING A LEAD PURSUIT COURSE

This problem was undertaken for partial Master's thesis credit by Donald Spangenberg and William Banks. The programming was done by Charles Block of the MIT Instrumentation Laboratory using the "George" code (an algebraic system described in previous Summary Reports under Problem 108). It involved solving 25 simultaneous first-order differential equations.

This problem was an attempt to study the performance of a particular fire control computer, replacing the human pilot by a suitable pilot-response-function. This same problem was run on a REAC with a human pilot in the system. By observing the pilot's responses over many REAC runs, Spangenberg and Banks were able to derive some sort of pilot-performance-function that should simulate the pilot's responses. Although the programming was technically correct, the results were not what Spangenberg and Banks anticipated. More time was needed in examining some of the logic used in going from an analog-type simulation to a digital-type. However, since theses were due, further work could not be carried out. The conclusions that were drawn on this incomplete study can be found in an MIT Flight Control Laboratory report 7210-T20, "Response of the Human Pilot in a Simulated Day-Superiority Type Fighter", by Spangenberg and Banks.

C. Block
Instrumentation Laboratory

287 D. SAMPLED-DATA CONTACTOR SERVOMECHANISM

The problem is to determine the response of a sampled-data contactor servomechanism which is disturbed by Gaussian noise. The system considered has no input other than the Gaussian noise disturbance. Because of the noise, the system output at a given time is described by a list of possible system outputs with their associated relative probabilities. This list is called an output-distribution. Interest is centered on determining at sampling points the output-distribution and/or its variance.

The output-distribution at sampling points is calculated by the following three general steps:

1) approximations are made to reduce the number of possible system-outputs;

2) the problem of calculating the output-distribution is stated in matrix form;

3) the matrix problem is solved on WWI.

The three steps will be discussed in order.

The number of possible system-outputs is reduced by the following two methods: 1) neglecting improbable system-outputs; 2) approximating the actual step response of the linear part of the system by a step response which reaches "steady-state" after a few sampling periods.

The output distribution computation can be stated in matrix form in the following manner. Consider a system-output vector V in a space whose coordinates are the possible system-outputs. The elements of V are then the probabilities of each of the possible system-outputs. The transformation of the output vector of one sampling point to the output vector of the next sampling point can be viewed as a process of multiplying the output vector by a matrix of transition probabilities. For a system with no input other than a stationary Gaussian noise disturbance, the transition matrix is constant.

WWI is used to multiply the transition matrix by the successive output vectors.

The responses of two sampled-data contactor servomechanisms have been obtained on WWI. The input to the program is the initial output distribution vector, the transition matrix, and the system-output corresponding to each vector. The procedure was coded by G. Mahoney of the MIT Digital Computer Laboratory. The results of this problem have been included in an S.M. thesis submitted by D. Chesler to the MIT Electrical Engineering Department.

D. Chesler
Electrical Engineering

288 N. ATOMIC WAVE FUNCTIONS

Electronic wave functions for atoms and molecules (for states of arbitrary symmetry) can be obtained to arbitrary accuracy by a method which consists of three relatively independent stages of calculation.

Stage A - choice of some finite set of single-electron functions, η_a and evaluation of all possible one- and two-electron integrals over this set. The integrals are matrix elements of operators occurring in the many-electron Hamiltonian.

Stage B - calculation of expansion coefficients of a set of orthonormal single-electron functions ϕ_α.

Stage C - calculation of configuration interaction effects and resolution of degeneracies in the variational matrix for the many-electron Hamiltonian.

If Stage B is carried out, with certain modifications which are too complicated to explain here, Stage C is greatly simplified. Techniques of group representation theory and perturbation methods can be used. The actual amount of calculation required is very small compared with Stages A and B.

The essential difference between atomic and molecular calculations is that in the atomic case there exists a set of basic functions η_a, the analytic Slater orbitals, which lead to rapid convergence in expansion of the self-consistent ϕ orbitals, and for which all integrals can be evaluated in closed form. No class of functions is known which has both these properties in the molecular case.

Programs are available at present which carry out Stages A and B for atomic wave functions. These are not yet in their most efficient form and some further programming is needed to join them into a single unit. Dr. R. K. Nesbet of the Solid State and Molecular Theory Group has programmed the calculation of integrals, Stage A for atoms, and the program for transforming integrals under Stage B. These programs are described in detail in the Quarterly Progress Report, Solid State and Molecular Theory Group, MIT, April, 1955.

In this problem programs developed under Problems 144, 218 and 234 are being used

to calculate electronic wave functions, with extensive configuration interaction, for the ^3P states of C, Si, and Ge.

R.K.Nesbet
Solid State and
Molecular Theory
Group

289 C. HEAT TRANSFER THROUGH HIGH-SPEED LAMINAR BOUNDARY LAYERS

In aeronautics, the effects of the viscosity and heat conductivity of air are generally considered to be confined to a thin layer of fluid, called the boundary layer, adjacent to the aircraft surface. In this region, certain terms in the Navier-Stokes equations and in the energy equation for a viscous, heat-conducting fluid may be neglected and the flow is governed by the boundary layer equations:

(1) $$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0$$ (continuity)

(2) $$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right)$$ (x-momentum)

(3) $$\frac{\partial p}{\partial y} = 0$$ (y-momentum)

(4) $$\rho u \frac{\partial h}{\partial x} + \rho v \frac{\partial h}{\partial y} = u \frac{\partial p}{\partial x} + \frac{\partial}{\partial y}\left(\frac{\mu}{Pr} \frac{\partial h}{\partial y}\right) + u\left(\frac{\partial u}{\partial y}\right)^2$$ (energy)

together with appropriate boundary conditions at the outer edge of the layer and at the wall, an equation of state and equations for μ and Pr as functions of the state of the air. In these equations, applicable to two-dimentional flows, the symbols are defined as follows:

x	co-ordinate in the wall along the direction of the free stream
y	co-ordinate normal to the wall
u	velocity component along x
v	velocity component along y
ρ	density
p	pressure
h	enthalpy
Pr	Prandtl number
μ	viscosity

Exact solutions have been obtained only for special classes of external flows and wall boundary conditions, usually with simplifying assumptions about the variation of air properties. For practical problems integral methods are often used in which the equations are satisfied only on the average across the boundary layer. The average values of mass flux, momentum flux, energy flux, etc., are represented by certain boundary layer thicknesses. Each thickness represents a term in an equation obtained by an integration of either equation (3) or (4) with respect to y across the layer, followed by some manipulation.

$$\theta = \int_0^\infty \frac{\rho u}{\rho_e u_e}\left(1 - \frac{u}{u_e}\right) dy$$

and a convection thickness

$$\delta_c = \int_0^\infty \frac{\rho u}{\rho_e u_e} \left(\frac{h - h_e}{h_w - h_e}\right) dy$$

where $(\ )_e$ refers to conditions in the free stream and $(\ )_w$ to conditions at the wall.

These quantities may be evaluated if the velocity and enthalpy profiles in the boundary layer and their relative scale, or thickness ratio, are given. It has been found that the various profiles occurring in the known exact solutions belong to one-parameter families - one for velocity and one for enthalpy - and it is generally assumed that the profiles in completely general flows belong to the same families.

Four equations are needed in general to calculate the growth of a boundary layer with heat transfer. Integral equations obtained from (3) and (4) describe the growth of θ and δ_c if the velocity and enthalpy profiles are known. To obtain the two parameters defining the latter, two additional equations are needed. In some methods they are obtained from the original differential equations evaluated at the wall; in others new integral equations are used, obtained by first multiplying the differential equations by u or y and then integrating.

An integral method is being developed at the Naval Supersonic Laboratory which involves essentially a new specification of the one-parameter family of enthalpy profiles as a fixed profile for all flows with isothermal walls on which a modifying profile may be superposed for flows with non-isothermal walls. The enthalpy profile parameter is then just the ratio in which these two profiles are combined. A new integral equation had to be developed for calculating the value of this parameter at any station along the surface from the given flow conditions. Actually two such equations were obtained, multiplying equation (4) first by u and then by y before integrating, since it was not known in advance which would prove more suitable. Four new thicknesses analogous to δ_c were introduced:

$$G(m,\Delta) = \int_0^\infty \left(\frac{\rho u}{\rho_e u_e}\right)^2 \left(\frac{h - h_e}{h_w - h_e}\right) dy$$

$$F(m,\Delta) = \int_0^\infty \frac{y}{\theta} \frac{\rho u}{\rho_e u_e} \left(\frac{h - h_e}{h_w - h_e}\right) dy$$

$$\pi(m,\Delta) = \int_0^\infty \frac{\theta^2}{u_e} \frac{\partial^2 u}{\partial y^2} \left(\frac{h - h_e}{h_w - h_e}\right) dy$$

$$\Gamma(m,\Delta) = \frac{u_e \theta \rho_e}{\mu} \int_0^\infty \frac{v}{u_e} \left(\frac{h - h_e}{h_w - h_e}\right) dy$$

Given either the isothermal or the modifying enthalpy profile, each of these integrals (as well as δ_c) is a function of the velocity profile parameter, m, and the thickness ratio of the velocity and enthalpy profiles, Δ. For each of 10 velocity profiles, values were needed for 15 thickness ratios. A total of 1500 numerical integrations were required.

These integrations were performed on the Whirlwind computer using the trapezoidal rule. The ten velocity profiles and two enthalpy profiles were fed into the computer in tabular form. The tabular interval of the velocity profiles was used as the interval for integration. Since the thickness ratio varied, the value of the enthalpy in general had to be interpolated in the stored table.

The integrations have been completed and work on the integral method is proceeding. The enthalpy profile modifying function was originally derived from the exact solution where the temperature potential across the boundary layer is decreasing in the streamwise direction. This function may or may not be satisfactory for flows with increasing temperature potential. If it is not, a new function will be derived, requiring a further 750 integrations.

J.A.F.Hill
Naval Supersonic
Laboratory

290 N. POLARIZABILITY EFFECTS IN ATOMS AND MOLECULES

The general problem is the calculation of the distortion produced on electronic wave functions for atoms under the influence of a variety of applied electrostatic fields and the subsequent use of this information to construct accurate electronic wave functions for molecules. There have been a number of programs written for Whirlwind which bear closely on this problem and the general aim is to utilize various combinations of these programs for production runs to obtain the large amount of numerical data required.

The work to date and that contemplated in the near future has been solely concerned with the atomic part of the problem. For this problem the most easily manageable set of basis functions in which to expand the one-electron wave functions is

$$r^{A+\ell} e^{-ar} Y_\ell^m (\theta,\varphi)$$

where A, a, m, ℓ are arbitrarily chosen parameters. Various combinations of these parameters have been chosen and sets of basis functions have been built up to describe the polarization of the following atoms and ions in a uniform field:

$$H^-,\ H_e,\ L_i^+,\ B_e^{+2},\ B^{+3},\ C^{+4},\ F^-,\ N_e,\ N_a^{+-},\ M_g^{+2},\ A_e^{+3},$$

$$C\ell^-,\ A,\ K^+,\ \text{and}\ C_a^{+2}.$$

Similar sets of basis functions have been set up to describe the distortion of the electronic wave function under the action of a point charge field for H^-, L_i^+, and F^-.

There are two stages in the calculation of these atomic wave functions and energies which require extensive numerical work. There are first, the computation of atomic one- and two-electron integrals between the various basis functions and secondly, the algebraic transformation of these integrals. The majority of the integrals (those for the free atom) are being obtained from Dr. R. K. Nesbet's atomic integral program which has been described in these Progress Reports and in those of the Solid State and Molecular Theory Group. There are sufficiently few integrals involving the perturbing field so that these have been done by hand computation and much of this work has been carried out by the R.L.E. Joint Computing Group. The second part involves a transformation program written by R.K.Nesbet (see Summary Report No. 41, p. 68, Problem 234) and the mechanization of the Roothaan scheme programmed by Dr. A. Meckler and R.K.Nesbet (see description in previous reports). It is expected that runs using a combination of all these programs simultaneously will soon be made.

L.C.Allen
Solid State and
Molecular Theory
Group

291 B. DYNAMIC BUCKLING

This problem is concerned with the response of structural columns to compressive end loadings which are applied very rapidly and which vary in time. The response may be elastic or plastic, the latter case being studied with the aid of WWI. The equations to be solved are a set of coupled ordinary differential equations of second order. The dependent variables are the coefficients of the normal modes of vibration of the structure, which are coupled in the plastic case but not in the elastic case. The Kutta-Gill method is being used to solve these equations.

Two programs have been used so far, both being of a preliminary nature. They have served to acquaint the programmer with the machine and to define the spacing of the independent variable which will give sufficiently accurate results. The second solution obtained pointed out a problem of slow convergence which is inherent in the mathematical work. The mathematics is presently being revised to correct this trouble.

R.E.Jones
Civil Engineering

292 A. COURSE 6.535, SPRING 1955 PRACTICE

Course 6.535, "Introduction to Digital Computer Coding and Logic" was given in the Spring term of 1955 by Mr. Dean N. Arden. Each student was required to solve one of the

following problems:

1. program and code a routine for the solution of a system of simultaneous linear equations by the Crout technique;

2. code two routines for the solution of a differential equation by different numerical methods and compare the results;

3. code a routine for the economization of a power series and compare the accuracy of the result with that of the power series truncated to the same order.

About 95 per cent of the students successfully completed the assignment.

293 C. ROLLING BEARINGS

The computer is to be used to solve the equations of motion of the rolling elements. Eight transcendental equations involving eight unknowns have been derived considering applied thrust load, inner ring speed, centrifugal force of rolling elements and normal and fractional forces in the contact zone. The direction and magnitude of the friction force in the contact zones are established by the relative slip, coefficient of friction and the local contact pressure.

The program has been written and is in the testing stage. Extensive use is made of library subroutines including those for minimizing sum of squares by the gradient method, the Gauss quadrature method, and a new cube root routine.

B. Riskin
Digital Computer
Laboratory

294 C. WIND TUNNEL DATA REDUCTION

The objective of the program was to see how the Whirlwind computer could be used to reduce data taken in the Naval Supersonic Wind Tunnel. In this particular example, forces and moments (3 components) were measured by strain gages mounted inside the model. The strain gage output at present is measured, in millivolts, by self balancing potentiometers whose output in digital form is automatically recorded on IBM punched cards. The data reduction process involves converting the potentiometer readings to force and moment coefficients by multiplying by calibration constants and referring these coefficients to axes which are fixed in space and do not move with the model.

The program was coded for the CS II computer with the output (run number, corrected angle of attack, dynamic pressure, base pressure coefficient, balance chamber pressure coefficient, drag coefficient, lift coefficient and pitching moment coefficient) recorded on magnetic tape. In addition, the machine was programmed to plot angle of attack, drag coefficient and pitching moment coefficient all as functions of lift coefficient. The desired results were obtained for three runs. During each run, the angle of attack varied through about 10 values.

Due to the method used in feeding data to the computer, unwanted tape numbers appeared between each row of tabulated data and on the plots so that a different method of storing the data would be used in future computations. Otherwise the program was successfully completed and indicated that the machine required about eight seconds per data point (a "data point" being all of the data at one angle of attack). Although more efficient programming could reduce this time slightly, it should still be a representative figure for more complicated programs (more components). All of the data from a good eight-hour shift of wind-tunnel time (about 20 runs, or 200 data points) could thus be reduced in about twenty-five minutes.

L. Schindel
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1. SYSTEMS ENGINEERING

Revisions in the Marginal Checking Procedures for the Drum System

The programmed-marginal-checking facilities have been expanded to include additional terminal equipment. Previously, this equipment was checked by taking manual margins during specially assigned maintenance periods. In order to include the drum equipment in the daily programmed-marginal-checking routines, it was necessary to modify the marginal-checking equipment. A check program cycle for this type of terminal equipment was necessarily long compared to the existing voltage variation cycle. It is now possible to select the marginal-checking equipment in a special mode which will hold a preset excursion for an amount of time determined by the program.

A consolidated test program containing nine routines has been written for the drum system. This program completely checks the equipment with a minimum amount of redundance. Special care was taken in choosing program techniques and in assigning variation lines in an effort to reduce the amount of time necessary to perform the checks. The considerable reduction in time gained by this programming effort made it practical to include the program as part of the daily marginal-checking routine. The drum system, containing approximately 5500 cathodes, is now checked in one half of the hour scheduled daily for system maintenance.

Analysis of Performance Records for the Whirlwind Computer System

In September 1954 the procedures for gathering and evaluating performance data on the computer system were somewhat revised. This was done to permit more comprehensive analyses of system reliability with particular emphasis on interrupting failures. A description of these procedures as well as an analysis of the data gathered over a 20-week period ending 10 February 1955 was published in Memorandum 6M-3410.

Several figures are required to adequately describe the reliability of an electronic system. In general, system reliability is reflected in the amount of scheduled down time required for preventive maintenance. Since the amount of down time for different types of failures varies widely, the frequency of such failures is also an important factor in describing system reliability. In the following table such reliability figures are given. Results for the first 20-week period as reported in Memorandum 6M-3410 are listed along with similar data for the succeeding 3 months.

	28 Sept. 1954 to 10 Feb. 1955	11 Feb. 1955 to 19 May 1955
Total computer operating time	2675 hours	1923 hours
Total lost time	92.7 hours	65.2 hours
Percentage operating time usable	96.5 percent	96.6 percent
Average uninterrupted operating time between failure incidents	10.6 hours	10.9 hours
Failure incidents per 24-hour day	2.17	2.12
Average lost time per incident	22.8 minutes	23. minutes
Average preventive maintenance time per day	1.25 hours	1.5 hours

2. PUBLICATIONS

Project Whirlwind technical reports and memoranda are routinely distributed to only a restricted group known to have a particular interest in the Project, and to ASTIA (Armed Services Technical Information Agency) Document Service Center, Knott Building, Dayton, Ohio. Requests for copies of individual reports should be made to ASTIA.

The following is a list of memoranda published by the Scientific and Engineering Computations Group during the past quarter.

No.			
DCL-66	List of Memos on Programming and Coding for WWI	4-4-55	S and EC Group
DCL-69	S and EC Operator's Check List	4-4-55	J. Thompson
DCL-71	Notes on Tape Room Operating Procedure	4-29-55	M. Solomita, H. Bello, and F. Shaw
DCL-73	Treatment of Flexo Coded Characters by The Comprehensive System (Revision of Table)	5-5-55	J. M. Frankovich
DCL-76	The Availability of Floating Address Values Following CS Conversions	5-20-55	J. M. Frankovich
DCL-77	Index of Subroutines Available for the WWI Computer	6-1-55	S and EC Group

3. VISITORS

Tours of the WWI installation include a showing of the film "Making Electrons Count", a computer demonstration, and an informal discussion of the major computer components. During the past quarter, 9 groups totalling 188 people visited the computer installation. Included in these groups were:

April 28	Newton High School
May 4	M.I.T. Biology Department
May 10	Northeastern University
May 11	Operations Research Seminar
May 26	Class in "Introduction to Digital Computers - Coding and Logic", M.I.T.
June 16	Professor Gregory's Summer Session class, M.I.T.
June 24	Professor Hildebrand's Summer Session class, M.I.T.

The procedure of holding Open House at the Digital Computer Laboratory on the first Tuesday of each month has continued during this period. Three groups totalling 58 persons visited the Laboratory at the Open House demonstrations. These persons represented members and friends of the M.I.T. community, Boston Safe Deposit and Trust Co., Raytheon, Garland Jr. College, Natick High School, Laboratory for Insulation Research, John Hancock Life Insurance Co., Signal Manufacturing Co., and the Massachusetts Memorial Hospitals.

During the past quarter there were also 78 individuals who made brief tours of the computer installation at different times. Some of the companies represented by these individuals are Chance-Vought Aircraft; Bridgestone Tire Co. and Oktsu Tire Co. of Japan; Godfrey L. Cabot Co.; Institute de Statistique, Paris; British Grain and Seed Co.; U. S. Army Signal Corps; Whirlpool Co., Link Aviation Co.; Monsanto Chemical Co.;

I.C.I., Ltd., England; Gulf Research and Development Co., Allegheny Refining Co.; Remington Rand Corp.; Westinghouse Electric; Bell Telephone Laboratories; The British Milk Marketing Board; The British Tabulating Co.; and Philips, N.V., Holland.

PERSONNEL OF THE PROJECTS

MACHINE METHODS OF COMPUTATION AND NUMERICAL ANALYSIS

Faculty Supervisors:

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Samuel H. Caldwell	Electrical Engineering
Sidney D. Drell	Physics
Jay W. Forrester	Electrical Engineering
Francis B. Hildebrand	Mathematics
John A. Hrones	Mechanical Engineering
George B. Thomas, Jr.	Mathematics

Research Associate:

Bayard Rankin	Mathematics

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Leo Sartori	Physics
Aaron Temkin	Physics
Marius Troost	Chemical Engineering
Arnold Tubis	Physics
Jack L. Uretsky	Physics
Keeva Vozoff	Geology and Geophysics

PROJECT WHIRLWIND

Staff Members of the Scientific and Engineering Computations Group at the Digital Computer Laboratory.

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