MACHINE METHODS OF COMPUTATION
and
NUMERICAL ANALYSIS

QUARTERLY PROGRESS REPORT NO. 15
MARCH 15, 1955

and

PROJECT WHIRLWIND
SUMMARY REPORT NO. 41
FIRST QUARTER 1955

Submitted to the

OFFICE OF NAVAL RESEARCH
Under Contract N5ori60
Project NR 044-008

Project Nos. DIC 6915 and 6345

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TABLE OF CONTENTS

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 N5ori60.

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 MIT 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. This speed is higher than general scientific computation demands at the present state of the art, but is needed for control and simulation studies.

PART I

Machine Methods of Computation and Numerical Analysis

1. GENERAL COMMENTS

During the fall and winter the contacts between the project staff and others working in the field of numerical analysis and machine computation have increased in frequency and broadened in scope. The Discussion Group on Numerical Analysis to be mentioned in section 3, has stimulated the interest and participation of a number of members of the Mathematics Department. Other research projects finding a need for machine calculation, have come to depend on this project for help in finding how best to use computing equipment. The Solid-State and Molecular Theory Group under Professor J. C. Slater, has been using Whirlwind and other computing equipment to an increasing extent. Corbato, a member of the Machine Project, has been spending much of his time with Slater's Group, helping various members code their problems and working out appropriate computing methods. Uretsky, Sartori and Rotenberg have been working with members of the Theoretical Group of the Research Laboratory for Nuclear Science and Engineering, applying machine techniques to numerous problems in this field.

There has also been close contact with the staff of the Operations Research Project, particularly in the study of problems of Linear Programming and techniques for their solution. Joint seminars have been held. Some of the Whirlwind staff have been examining the simplex method and other techniques for obtaining solutions to linear programming problems. John D. C. Little, who transferred from this project to the Operations Research project last year, completed the solution to a dynamic programming problem this fall, using Whirlwind to obtain numerical results. Other groups, both in engineering and in pure science, have received advice and help in connection with their computing or data handling problems.

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

A STUDY OF THE BASIC PROBLEM OF NUMERICAL ANALYSIS EXPRESSED IN THE LANGUAGE OF COMPUTING MACHINES

The following report introduces a new project that has developed partly out of the discussion group on numerical analysis referred to under Group Activities in the last quarterly report. The discussion group is still continuing (as recorded in section 3 of the present quarterly) and will be used as a place to work over and extend the ideas that are presented here.

The question of what aspects of numerical analysis are most important for improving machine methods is not much different from the question of what are the essential aspects of numerical analysis. The reason for this is that numerical analysis is to be regarded as a study of computational methods, or methods for solving problems that ultimately yield numbers, and as such is directed toward computing machines. Of course, the mathematician need not distinguish between a calculational procedure that is carried out by hand and one that is carried out mechanically or electronically; both are procedures for a machine. Therefore, it seems only realistic that numerical analysis should be studied in conjunction with the logic of computing machines and that the problems of numerical analysis should be couched in the language of the computing machines for which they are destined.

This observation should be balanced with the realization that the language of mathematics, as opposed to the language of machines, is not highly adapted to computational procedures - except in the most simple cases of arithmetic. The language of mathematics in which most numerical analysis is done accomodates concepts of limits, for example, which are present in computations only in an approximate sense. On the other hand, the concept of time required to carry out a mathematical operation, or the concept of decision (so essential to iteration procedures) are only indirectly accomodated by the usual tools of mathematics and at best carry a very different significance in the fields of abstract and applied mathematics.

Thus, while numerical analysis has an affinity for computing machines, the language in which it is studied is in some ways foreign to them. There are two unfortunate results: first, the basic problems of numerical analysis are at times obscured or complicated, and, second, all results must be translated into the language of machines. In the present paper there is an attempt to rectify this situation by defining in the language of machines the most basic problem of numerical analysis. We will later attempt to outline some techniques for solving the problem. Such an outline can only be tentative and any ideas in it can at best be exemplary. It should also be emphasized that the "basic problem of numerical analysis" is to some extent born of a subjective judgement.

In the language of computing machines, a numerical solution to a mathematical problem is a collection of parameter values and a sequence of instructions. The parameters and instructions determine an output in the form of a set of numbers. The numerical solution to a particular problem solved on a particular machine has, of course, the same ingredients, but the instructions must be specialized to the machine and the output must be close in some sense to a desired set of numbers. (It is unrealistic to speak of exactness of an output to a desired set of numbers, because only in rare cases can a numerical solution be an exact solution to a problem.) Having defined a numerical solution, it is clear that there are many such for each mathematical problem, because there are many sequences of instructions with outputs that are within a certain degree of closeness to a desired set of numbers. The flexibility that permits a multiplicity of numerical solutions comes, first, from the fact that many sequences of instructions give the same output and, second, from the fact that the same output is not even required in order for two numerical solutions to satisfy a given problem. Thus if one attaches a measure of time to each sequence (the length of time for the machine to perform the sequence) and a measure of accuracy (the closeness of the output to a desired set of values) there will be two quantitative ways to compare the many numerical solutions to a given problem.

It is proposed here that numerical analysis is not chiefly concerned with finding a possible numerical solution among a great multiplicity. The basic problem of numerical analysis is to find the fastest and most accurate out of a set of possible numerical solutions. This statement will now be made more precise.

It is first necessary to define mathematically what is meant by a machine, M. Let $P = (P_1, P_2, \ldots, P_n)$ be a sequence chosen from the space, $\mathcal{P}$, of sequences of real valued parameters. P represents the input data or other parameters initially held in the memory of the machine. Let $I = (I_1, I_2, \ldots, I_m)$ be a sequence chosen from the space, $\mathcal{I}$, of sequences of instructions. The instructions are assumed to pertain to the machine M. Let O be a mapping of the pairs (P, I) onto the space of sequences $(O_1, O_2, \ldots, O_r)$ of real numbers. O (P, I) is the output determined by the parameter set P and the instructions I. Let T be a mapping of the pairs (P, I) onto the positive real axis. T (P, I) is the time required for the machine M to perform the sequence I, assuming that the parameters in the machine's memory are P. Now for mathematical purposes, the machine M is completely specified by the cross-product space $\wp \times \vartheta$ and the two mappings defined on this space, O and T. Thus, we will write:

$$M \equiv (\wp \times \vartheta, O, T).$$

The points (P, I) in the space $\wp \times \vartheta$ may be described as possible numerical solutions to a mathematical problem. Of course, one solution may be better than another for a particular problem, and we ultimately want to say in what sense a possible numerical solution is optimal for a particular mathematical problem. Therefore, we must now define an entity which characterises each mathematical problem for the machine M. This is determined by two components, a possible solution (P_o, I_o) whose output $O(P_o, I_o)$ is a desirable set of numbers for the mathematical problem, and a distance function, δ, defined on the space of all possible pairs of outputs $[O(P, I), O(P', I')]$. The entity, itself, is a real valued function, D, defined on the cross-product space $\wp \times \vartheta$:

$$D(P, I) = \delta[O(P, I), O(P_o, I_o)] .$$

It is necessary to assume that (P_o, I_o) is known in order to state the basic problem of numerical analysis in the language of machines. This assumption is justified, because numerical analysis is chiefly concerned with something deeper than finding a set of numbers that approximately satisfy the restrictions imposed by a mathematical problem. After all, it is not difficult, if there are no practical limitations, to specify a sequence of instructions which yield numbers closely approximating an integral of a function, the derivative of a function, the solution of an integral equation, or the solution of a differential equation. Thus, (P_o, I_o) may be viewed as the solution to a mathematical problem translated into machine language without any regard for practicality, such as speed of convergence, number of iterations involved, etc.. The distance function may be viewed as a criterion for judging how a solution that may be more practical than (P_o, I_o) compares in accuracy to (P_o, I_o).

After these considerations, the basic problem of numerical analysis appears to have the following two forms:

Form I: Given the machine $(\wp \times \vartheta, O, T)$, the mathematical problem D, and the positive number D_o, to find (P', I') such that $T(P', I') = \min_{S_{D_o}} T(P, I)$, where $S_{D_o} = \{(P, I): D(P, I) < D_o\}$.

Form II: Given the machine $(\wp \times \vartheta, O, T)$, the mathematical problem D, and the positive number T_o, to find (P", I") such that $D(P'', I'') = \min_{S_{T_o}} D(P, I)$, where $S_{T_o} = \{(P, I): T(P, I) < T_o\}$.

If the minimums do not exist or are not unique, of course the above forms must be slightly modified.

It should be pointed out that in any practical case, the outputs O(P, I), $O(P_o, I_o)$ will not be known to the numerical analyst when he attempts his problem of optimizing. Nevertheless, it will be shown later how D (P, I) can be determined once δ and (P_o, I_o) are specified and how the minimization can be carried out at least approximately. It is also true, practically, that the time T(P, I) will not be known, though ordering relations of the type, T(P,I) < T(P', I'), will in general be known. In fact, though the above forms of the basic problem appear to be fairly familiar, it is the lack of knowledge about O and T that identifies the problem with machines and numerical analysis.

Bayard Rankin

EVALUATION OF THE EXPLICIT DIFFERENCE FORMULA FOR A PARABOLIC DIFFERENTIAL EQUATION

The present report is concerned with the explicit difference approximation to the diffusion equation

$$(1) \qquad \frac{\partial^2 \psi}{\partial x^2} = \frac{\partial \psi}{\partial t}, \quad 0 \le x \le 1 \text{ and } 0 \le t ,$$

in the form of

$$(2) \qquad \psi_{j,k+1} = r_f \psi_{j-1,k} + (1 - 2r_f)\psi_{j,k} + r_f \psi_{j+1,k}$$

where r_f is the ratio $\Delta t/\Delta x^2$ for the formula which may be different from the real time ratio r. The exact solution for equation (1) is in the form of

$$(3) \qquad \psi_{x,t} = \psi_{x,\infty} + \sum_{n=1}^{\infty} C_n e^{-\alpha_n^2 t} (\tan\alpha_n \sin\alpha_n x + \cos\alpha_n x)$$

and that for equation (2) is

$$(4) \qquad \psi_{j,k} = \psi_{j,\infty} + \sum_{n=1}^{M+1} D_n \lambda_n^k (\tan M\beta_n \sin\beta_n j + \cos\beta_n j)$$

$$\text{where} \quad \lambda_n = 1 - 2r_f(1 - \cos\beta_n)$$
$$k = t/\Delta t$$
$$j = x/\Delta x$$

and β_n and α_n are characteristic values depending on the boundary conditions. A method to optimize the explicit approximation for coarse grid network (that is, $M = 1/\Delta x$ is small) is explained in the Quarterly Progress Report No. 13 (September 15, 1954). Initial conditions are $\psi_{x,0} = 0$. The boundary conditions are $\frac{\partial}{\partial x}\psi_{1,t} = 0$

and (I) $\psi_{0,t} = 1$

(II) $\frac{\partial}{\partial x}\psi_{0,t} = -1$

(III) $\psi_{0,t} - Q\frac{\partial}{\partial x}\psi_{0,t} = 1$ where $Q = \frac{1}{3}$, 1, and 3.

The optimized parameters r_f, r, and $\psi_{0,0}$ or $\psi_{-1,0}$, the corner values for cases I and II are given in Quarterly Progress Report No. 14 (January 1, 1955).

For case III, the second order difference form for the boundary condition is

$$(5) \qquad \psi_{0,k} - \frac{QM}{2}(\psi_{1,k} - \psi_{-1,k}) \doteq 1 .$$

The β_n's in (4) have all the M+1 values instead of M. The characteristic values are the roots of the transcendental equation

$$(6) \qquad MQ_f \tan M\beta_n \sin\beta_n = 1 .$$

The M+1th value is $\beta_{M+1} = \pi + i\gamma$ which is complex. Similarly, the α n's in (3) are the roots of the transcendental equation

$$(7) \qquad Q\alpha_n \tan\alpha_n = 1$$

Since α n's from (7) and β_n's from (6) have no simple relationship, direct comparison of (3) and (4) shows that not only the excitation modes, C_n and D_n, and the decaying modes, $e^{-\alpha_n^2 t}$ and λ_n^k are different but also the space modes are different. The optimization scheme is to make

(1) $D_1 = C_1$ by choosing $\psi_{-1,0}$

(2) $\lambda_n^k = e^{-\alpha_n^2 r k/M^2}$ for n = 1 and 2 by choosing r_f and r

and (3) $M\beta_1 = \alpha_1$ by choosing Q_f different from Q in equations (6) and (7).

The merits of this optimization method are evaluated by comparing results of the same condition with $r = \frac{1}{6}$ [1] and with the exact analytical solution. Step by step calculations are made by the Whirlwind Computer.

Results of the cases I and II so far show that the excitation modes are more important when r is in the neighborhood of $\frac{1}{6}$. Both the present method and the $r = \frac{1}{6}$ with a corner value adjustment yield similarly good results and are both superior to cases where r is choosen to be other values. For case III with $Q = \frac{1}{3}$, the present method gives many times better results.

Results are still being completed and studied. Investigation also includes application of the step responses to varying boundary conditions, such as $\psi_{0,t} = \sin 2\pi t$, by the method of superposition. Details of the complete results will be available in the final report in the coming Quarterly.

Stability criterion can be shown by equation (4), the explicit formula will decay toward the steady state value when $|\lambda_*| \leq 1$. In other words

(8) $r \leq 1/(1 - \cos\beta_n)$.

The critical value lies on the highest mode. Thus, for case I where ψ is prescribed,

$$\beta_M = (1 - \frac{1}{2M})\pi \quad \text{and} \quad r \leq \frac{1}{2}^{+}$$

for case II where $\frac{\partial\psi}{\partial x}$ is prescribed,

$$\beta_M = \pi \quad \text{and} \quad r \leq \frac{1}{2}$$

and for case III where $\psi - Q\frac{\partial\psi}{\partial x}$ is prescribed,

$$\beta_{M+1} = \pi + i\gamma \qquad \text{and} \quad r \leq \frac{1}{1+\cosh\gamma} = \frac{1}{2}^{-}$$

In the limit where $M \rightarrow \infty$, stability criterion for all cases $\rightarrow \frac{1}{2}$.

In the case of heat transfer in a finite slab $0 \leq x \leq 1$ when temperature is prescribed on the boundary, the explicit formula of finite grid network is stable for r values greater than $\frac{1}{2}$ depending on the grid size; but when a heat transfer film coefficient is present, the formula is stable only for r values less than $\frac{1}{2}$. This latter result checks with Fowler [2] who derived the similar result by contour integration method.

Andrew T. Ling

References:

[1] W. E. Milne, "Numerical Solution of Differential Equations", John Wiley, N.Y., 1953, p. 122.
[2] C. M. Fowler, "Analysis of Numerical Solutions of Transient Heat-Flow Problems", Quart. Appl. Math. 3, 361-376 (1946)

CALCULATION OF NUMBERS OF STRUCTURES OF RELATIONS ON FINITE SETS

In group theoretic studies, the question has arisen, given a set of objects how many structures of relationships may be defined among members of the set? A general formula which yields, in principle, the answer to this problem is available, but even for small sets this formula involves extended calculations, practically demanding a high-speed machine for their accomplishment. Whirlwind I is at present being used to evaluate the formula for small sets.

To specify the problem precisely, consider a set of n objects. A dyadic relation among members of the set is specified completely by an nxn matrix of 1's and 0's, a one in the ij place indicating that element i bears the relationship to element j while a zero indicates the absence of such a relationship. Counting the number of structures of relations amounts simply to counting the admissable arrays of 1's and 0's in such a matrix. With no further restrictions, we see that the answer is 2^{n^2}, but in this figure of 2^{n^2} we have included many isomorphic structures which can be permuted into one another simply by renumbering the objects of the set. This then is the problem, how many nonisomorphic structures exist?

The possible numberings of the set are simply the n! permutations forming the symmetric group of order n! Consider the matrix transformation which occurs when such a permutation is effected on members of the set without altering the relational structure. Let the permutation be represented by π, renumbering object i with the label $i' = \pi i$. Then if the relational matrix is A, this permutation introduces a transformation, of the matrix A into a new matrix A'. Symbolically,

$$T_\pi A = A'$$

$$a_{ij} = a'_{\pi i, \pi j}$$

Thus any basic matrix pattern may be transformed into n! ostensibly different patterns by application of each of the n! induced transformations T_π. Of course some of these n! patterns may be repetitions of each other, for example the matrix all of whose elements are one transforms into itself under every T_π. If we list all the 2^{n^2} matrices and perform the n! transformations on each, we find the list partitioned into exclusive and exhaustive subgroups or "orbits". Every member matrix of one orbit may be obtained from every other member by applying a suitable T_π, whereas no member of a different orbit may be so obtained. These orbits are the abstract nonisomorphic structures.

Group theoretic reasoning yields the following expression for the number of orbits or structures of a general m-adic relation (the matrix becomes an m-dimensional array rather than 2-dimensional)

$$\mathrm{str}_n^m = \frac{1}{n!}\sum_{\pi} f(\pi)$$

where str_n^m is the number of structures of m-adic relations on a set of n elements. To define $f(\pi)$, look at the result of a given permutation π upon each of the 2^{n^m} relational arrays. Some of these arrays, as pointed out above are invariant under π, that is

$$T_\pi A = A$$

$f(\pi)$ is defined as the number of A's for which this holds true. The summation is then taken over the n! different π's. On the surface this formula would appear to involve inspection of all the n! transforms of the 2^{n^m} arrays, comparing the n^m elements of the transforms with the elements of the original arrays, hardly a feasible project. However Davis develops a version of the formula applicable to computation:

$$\mathrm{str}_n^m = \frac{1}{n!}\sum_{\tilde{\pi}} b(\pi)\, 2^{d_m(\pi)}$$

$$b(\pi) = n!\left(1^{p_1} p_1!\, 2^{p_2} p_2! \cdots n^{p_n} p_n!\right)^{-1}$$

$$d_m(\pi) = \sum_{r_1 \cdots r_m = 1}^{n} p_{r_1} \times \cdots \times p_{r_m} \frac{r_1 \times \cdots \times r_m}{c}$$

or in particular

$$d_2(\pi) = 2\sum_{h<k} p_k\, p_h\, (h, k) + \sum_{k=1}^{n} K p_k^2$$

c = least common multiple of $r_1, r_2 \ldots r_m$

(h, k) = greatest common divisor of h, k

There is still plenty of calculating involved in these formulas. Consideration of different π's has been reduced from all of the n! permutations to representatives, $\tilde{\pi}$, from each of the "conjugate classes" of permutations having similar disjoint cycle schemes

$$(p_1, p_2 \ldots p_n)$$

Where p_r is the number of cycles of length r in the permutation. (In a cycle, the first element is permuted into the second, the second into the third, the last into the first). Since the total number of objects is n, the p_r must fulfill

$$\sum_{r=1}^{n} r\, p_r = n.$$

Most of the p_r are zero. The total number of conjugate classes, or terms in the summation for str_n^m, is the number of partitions of n into integral summands. For n = 10 there are 42 terms for n = 20, 385. (Compare these figures with n!, the total number of permutations which is 3.6×10^6 for n = 10 and 2.4×10^{18} for n = 20.) The redundancy, or number of member permutations, of each conjugate class is b (π). f (π) has been replaced by $2^{d_m(\pi)}$ where $d_m(\pi)$ represents the number of "degrees of freedom" corresponding to a particular permutation. The number of degrees of freedom is the number of elements of the array A which one may choose at random and still be able to have $T_\pi A = A$. This number is definitely limited since in choosing, say, a_{ij} we must assign the same value to $a_{\pi i, \pi j}$ and in turn to $a_{\pi^2 i, \pi^2 j}$, etc. until we go through an entire cycle returning to a_{ij}. In the particular case of dyadic relations, m = 2, the computing formula for $d_2(\pi)$ includes a term for degrees of freedom in the off-diagonal elements and one for the degrees of freedom in the diagonal elements. Other formulas are available for special classes of dyadic relations, symmetric, reflexive, or antisymmetric.

This problem is interesting from the programming standpoint in that it requires exact answers which are very large integers, far exceeding the 15-bit capacity of Whirlwind I. Operations must be conducted in integers with no round oft; in division, remainders must be kept. The program is arranged to develop each of the position schemes $(p_1, \ldots p_n)$ in logical order. From each partition follows b (π) and $d_m(\pi)$. Extensive use of the logical orders is necessary in the partition developments, and in efficient calculation of the sums for $d_m(\pi)$ which, as written contains about $n^2/2$ terms for an nxn matrix, but at most about n non-zero terms.

Because of the necessity of carrying very large numbers exactly and because upper bounds for the quantities involved vary by as much as the capacity of several whirlwind registers even within the calculations for one particular n, (for example upper and lower limits on b (π) one $n!/(n-1)$ and 1) and are in any case difficult to estimate, a flexible arithmetic routine has been provided which is capable of carrying out addition, multiplication, division, and shifting of multi-register positive numbers of arbitrary length. Operation with this routine will be very slow for two-register numbers, but unfortunately numbers as long as 8 registers may be encountered even for n =10.

The present calculations are limited to the calculation of the numbers of structures at dyadic relations, and will be carried to sets as large as time will permit; I hope to n = 15. The necessary routines are now being tested on Whirlwind I.

Reference: [1] R. L. Davis, Proc. Am. Math. Soc. 4, 486 (1953)

M. Douglas McIlroy

THE STABILITY OF THIN, SHALLOW ELASTIC SHELLS

The problem under consideration is that of the stability of a hyperbolic paraboloidal shell loaded by its own weight. Specifically we wish to find that load, p_o, which causes the shell to buckle. The equation of the shell is

$$z = C \frac{x}{a} \quad \frac{y}{b} \tag{1}$$

and the assumption of shallowness is that $\left(\frac{\partial z}{\partial x}\right)^2, \left(\frac{\partial z}{\partial y}\right)^2 << 1$.

The precise conditions of the problem being studied are:

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 complete solution of the general equations of shallow shell theory is [1]

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

where w is deflection in the z direction and F is the stress function. To test the stability of this solution we assume new solutions of the form

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

Substitute these into the differ ial equations and linearize the differential equations in terms of $\bar{w}$ and Φ. The equations which hcld are

$$\begin{aligned} \nabla^2\nabla^2 \Phi &= \frac{Eh2c}{ab} \frac{\partial^2 \bar{w}}{\partial x \partial y} \\ D\nabla^2\nabla^2 \bar{w} &= -\frac{2c}{ab} \frac{\partial^2 \Phi}{\partial x \partial y} + p_o \frac{ab}{c} \frac{\partial^2 \bar{w}}{\partial x \partial y} \end{aligned} \tag{4}$$

where h is the uniform thickness of the shell, E is the Modulus of Elasticity and D is the modulus of Flexural Rigidity. The boundary conditions are

$$\left.\begin{aligned} x &= 0, a \\ y &= 0, b \end{aligned}\right\} \quad \bar{w} = \nabla^2 \bar{w} = \Phi_{xx} = \Phi_{yy} = 0 \tag{5}$$

(4) and (5) then represent a characteristic value problem for p_o, the buckling load.

To find the buckling load we assume series expansions for w and Φ, satisfying the boundary conditions, as follows

$$\begin{aligned} \bar{w} &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \sin \frac{m\pi x}{a} \sin \frac{n\pi y}{b} \\ \Phi &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} B_{mn} \sin \frac{m\pi x}{a} \sin \frac{n\pi y}{b} + B_{oo}\, xy . \end{aligned} \tag{6}$$

Substitution of (6) into (4) leads to a doubly infinite set of linear homogenous equations in the A_{mn} and B_{mn}. P_o is a parameter in this doubly infinite set. We desire to find the smallest value of p_o which permits solution of the set by non-zero A_{mn} and B_{mn}. To obtain approximations to the desired p_o the series (6) will be terminated after a finite number of terms. The solution of this finite eigenvalue problem and the convergence of the solution to the true value of p_o will be investigated.

Anthony Ralston

References:

[1] E. Reissner, "On Some Aspects of the Theory of Thin Elastic Shells," Journal of the Boston Society of Civil Engineers (In Press)

MACHINE SOLUTION OF THE DIFFUSION EQUATION

The one dimensional diffusion (or heat) equation of the type

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[k(x) \frac{\partial u}{\partial x}\right] \quad ; \quad k(x) > 0 \quad \text{in} \quad 0 \le x \le L \tag{1}$$

with initial and boundary conditions

$$\begin{aligned} -k(x) \left.\frac{\partial u}{\partial x}\right|_{x=0} &= Q , \quad 0 < t \\ \left.\frac{\partial u}{\partial x}\right|_{x=L} &= 0 , \quad 0 < t \\ u(x,0) &\equiv 0 , \quad 0 < x < L \end{aligned}$$

where U is concentration (or temperature) (X has units of length and t has units of time) has a unique solution which can be put into the form

$$u(x,t) = \frac{Q}{L}\left[\int_0^x \frac{z-L}{k(z)}\, dz + t\right] + C - \sum_{n=0}^{\infty} C_n e^{-\lambda_n t} X_n(x) \tag{2}$$

where $$C = \frac{1}{L}\int_0^L \left(\int_0^z \frac{L - z_1}{K(z_1)}\, dz_1 \right) dz$$

and $$C_n = -\frac{Q}{L}\int_0^L \mathfrak{X}_n(z) \left(\int_0^z \frac{L - z_1}{K(z_1)}\, dz_1 \right) dz \Big/ \int_0^L \mathfrak{X}_n^2(z)\, dz \, .$$

The $\mathfrak{X}n$ are a complete set of orthogonal functions belonging to the associated Sturm-Liouville system:

$$\frac{d}{dx}\left[K(x) \frac{d\mathfrak{X}_n}{dx} \right] + \lambda_n \mathfrak{X}_n = 0$$

(3) $$\left.\frac{d\mathfrak{X}_n}{dx}\right|_{x=0} = \left.\frac{d\mathfrak{X}_n}{dx}\right|_{x=L} = 0$$

This solution is found by using the separation of variables method. First, assume the form

$U^{(1)} = R(X) + S(t) + C$ and satisfy the first two boundary conditions of (1). This will serve to determine a constants except C. This is the steady-state solution (that part of the solution which does not die out with time). Next use $U^{(2)} = X(x)\, \mathcal{T}(t)$ with the boundary conditions for (3) above plus the condition on $\mathcal{T}$: $\lim_{t \to \infty} \mathcal{T}(t) = 0$. This product form yields the solutions

$$C_n e^{-\lambda_n t} \mathfrak{X}_n(x).$$

These two solutions are then fitted together (using a type of Fourier expansion of R(x) in terms of Xn function) to satisfy the initial condition at $t = 0$. The constant c is determined from the fact that

$$\int_0^L u(z,t)\, dz = Qt.$$

(See Quarterly Progress Report No. 14).

Equation (2) is valuable for two reasons. First, it displays the steady state solution and second, it suggests when the transient has become insignificant. A simple approximate calculation showed this occurred when $t = O(L)$.

A number of cases have been solved analytically in the literature [1, 2]. When K is constant, $\mathfrak{X}n$ are sines and cosines; when K is linear in x, $\mathfrak{X}n$ are given in terms of modified Bessel Functions of zero order. Corresponding forms of K will produce Legendre polynomials, Legarre polynomials, etc.

An interesting case is when $K(O) = 0$. For instance $K(x) = x$. Thus, by the Laplace transform with respect to t equation 1 becomes

$$x \frac{d^2\bar{u}}{dx^2} + \frac{d\bar{u}}{dx} - s\bar{u} = 0$$

$$\left. x\frac{d\bar{u}}{dx}\right|_{x\to 0} = -\frac{Q}{s}\,, \qquad \left.\frac{d\bar{u}}{dx}\right|_{x=L=\infty} = 0\,,$$

where
$$\bar{u}(x,s) = \int_0^\infty e^{-st} u(x,t)\, dt\,.$$

The solution to this is readily found to be

$\bar{U} = \frac{2Q}{s} K_o(2\sqrt{sx})$ where K_o is the modified Bessel Function of zero order. The inverse transform then gives

$$u = Q\int_0^t \frac{1}{\tau} e^{-x/\tau} d\tau = -Q E_i(-x/t)\,.$$

Two cases of K(x) were solved on the IBM Card Programmed Calculator. The first was for a constant K. The cpc solved the transient region in a little over two hours using the difference equation (c):

$$U(x, t+k) = r\,U(x+h, t) + (1 - 2r)\,U(x, t) + r\,U(x-h, t)$$

where $r = \frac{Kk}{h^2}$, k = t spacing, h = x spacing. The h and k were started very small, then, as the calculation proceeded, h was doubled and k increased by a factor of 4 so as to keep the same difference equation throughout. The h was doubled in this manner 8 times. The final solution agreed with the steady state solution to within 0.1%.

The second case was solved using a K as shown in figure 1.

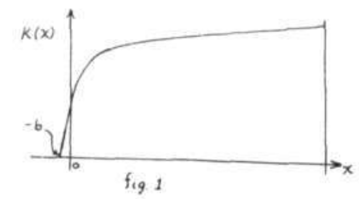

fig 1

$K(O) << K(L)$

$\frac{dK(0)}{dx} >> \frac{dK(L)}{dx}$

$K(-b) = O$

where $b << L$

In general, the solution U has a singularity at $X = -b$ which causes considerable difficulty in approximating the boundary condition at $X = O$, since any power series expansion on or near the boundary necessarily has a small radius of convergence. This seemed to suggest a variable spacing in the x direction (and consequently in the t direction). The difference equation corresponding to the point pattern in figure 2 is

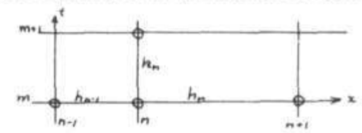

fig 2

(4) $$u_{n,m+1} = A_n u_{n-1,m} + B_n u_{n,m} + C_n u_{n+1,m}$$

where $A_n = k_n(2K_n - h_n K_n') \big/ h_{n-1}(h_n + h_{n-1})$, $C_n = k_n(2K_n + h_n K_n') \big/ h_n(h_n + h_{n-1})$,

and $B_n = 1 - k_n[2K_n - K_n'(h_n - h_{n-1})] \big/ h_n \cdot h_{n-1}$

where $K_n = K(x_n)$, $x_n = \sum_{i=0}^{n} h_i$; $\left.\frac{dK(x)}{dx}\right|_{x=x_n} = \left.K'(x)\right|_{x=x_n} = K_n'$.

It will be noticed that $An + Bn + Cu = 1$ and for local stability, all coefficients should be positive, consequently are equal to or less than one. Thus, we have the two conditions:

(5) $$h_n \le 2K_n / K_n' \,, \quad k_n \le h_n h_{n-1} \big/ [2K_n - K_n'(h_n - h_{n-1})].$$

For constant K and constant spacing these reduce to the well known stability conditions

$$K_n k_n / h_n^2 = Kk/h^2 \le 1/2 \,, \quad k > 0.$$

The first one in (5) places the limitation on h_n while the second, for given h_n and h_{n-1} gives the restriction on k_n. It was found that the x spacing satisfying the relation

$$(6) \qquad x_n = a(2^n - 1) \quad \text{for } 0 \le x_n \le L/2 \text{ and } a < b \text{ (in Fig 1)}$$

will conform to the first condition in (5) very well. Certainly, such a pattern is not unique and would depend on problem as well as the inclinations of the individual. This particular one worked very well for the KQ that was used. For the rest at the interval $(1/2)L \le X_n \le L$ constant spacing was used. Thus, for the first half interval

$$h_n = 2\, h_{n-1}$$

The kn spacing was chosen such that $k_n - 2\, k_{n-1}$ for the first half of the x -interval and constant k was used thereafter, i.e., for $x_n > (1/2)L$. The following figure 3 gives an abbreviated version of the overall point pattern used.

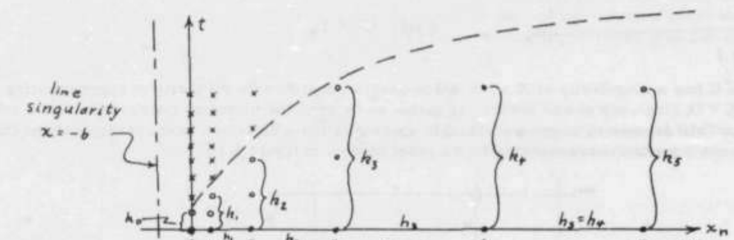

fig. 3

The dotted line represents the maximum extent one may predict into the region from the points on the bottom row (solid dots). The points calculated from the row are shown in open dots. The rest of the points are calculated using more immediate points (the open dots and previous crosses) and a completed line of points is eventually obtained across the entire interval (O,L).

The difference equations would be as follows

$$\begin{aligned}
U_{0,m+1} &= A_0 U_{-1,m} + B_0 U_{0,m} + C_0 U_{1,m} \\
U_{1,m+1} &= A_1 U_{0,m} + B_1 U_{1,m} + C_1 U_{2,m} \\
U_{2,m+1} &= A_2' U_{1,m} + B_2' U_{2,m} + C_2' U_{3,m} \\
U_{2,m+2} &= A_2 U_{1,m} + B_2 U_{2,m} + C_2 U_{3,m} \\
U_{3,m+2} &= A_3' U_{2,m} + B_3' U_{3,m} + C_3' U_{4,m} \\
U_{3,m+4} &= A_3 U_{2,m} + B_3 U_{3,m} + C_3 U_{4,m} \\
U_{4,m+8} &= A_4 U_{3,m} + B_4 U_{4,m} + C_4 U_{5,m} \\
U_{5,m+8} &= A_5 U_{4,m} + B_5 U_{5,m} + C_5 U_{6,m}, \quad etc.
\end{aligned}$$

where

$$A_n' = A_n/2, \quad C_n' = C_n/2, \quad B_n' = (1 + B_n)/2 .$$

The boundary condition at X = O may be approximated by

$$(8) \qquad U_{-1,m} = U_{0,m} + h_0 Q / K(0) .$$

The condition at X = L may be approximated by

$$U_{N-1,m} = U_{N+1,m}.$$

where $X_N \doteq L$.

Even with this short-cut of variable spacing the calculation time is very large due to the relatively dense columns of points for n = 0, 1, 2. This is especially true when relation (6) holds for a dozen or so points before constant spacing is applied as was the case actually used and described by figure 1. A further reduction in time may be had by combining the difference equations (7) in an appropriate manner. Thus the first equation with the above boundary condition at X = O is

$$U_{0,m+1} = h_0 Q/K(0) + (A_0 + B_0) U_{0,m} + C_0 U_{1,m}$$

and

$$\begin{aligned}
U_{0,m+2} &= h_0 Q/K(0) + (A_0 + B_0) U_{0,m+1} + C_0 U_{1,m+1} \\
&= h_0 Q/K(0) + (A_0 + B_0)\left[2h_0 Q/K(0) + (A_0 + B_0) U_{0,m} + C_0 U_{1,m}\right] \\
&\quad + C_0 \left[A_1 U_{0,m} + B_1 U_{1,m} + C_1 U_{2,m}\right],
\end{aligned}$$

or

$$U_{0,m+2} = a_0 + b_0 U_{0,n} + d_0 U_{1,m} + e_0 U_{2,m} ,$$

likewise

$$U_{1,m+2} = a_1 + b_1 U_{0,m} + d_1 U_{1,m} + e_1 U_{2,m} + f_0 U_{3,m}$$

where

$$\begin{aligned}
a_0 &= \frac{hoQ}{K(O)}(1 + A_0 + B_0) & a_1 &= A_1 \frac{hoQ}{K(O)} \\
b_0 &= (A_0 + B_0)^2 + A_1 C_0 & b_1 &= A_1 (A_0 + B_0) + B_1 A_1 \\
d_0 &= (A_0 + B_0)\, C_0 + C_0 B_1 & d_1 &= A_1 C_0 + B_1^2 + C_1 A_2' \\
e_0 &= C_1 C_0 & e_1 &= B_1 C_1 + C_1 B_2' \\
& & f_1 &= C_1 C_2'
\end{aligned}$$

One may proceed in this manner for $U_{o,m+4}$, $U_{o,m+8}$, $U_{1,M+4}$, $U_{1,m+8}$, $U_{2,m+8}$, ... as long as one likes. The coefficients will always be in terms of sums of products of preceding coefficients and the A, B, C. The resulting point patter may look like that in figure 4.

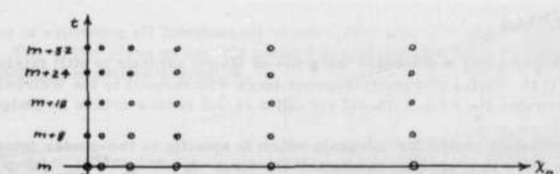

fig. 4

A good checking device may be had when calculating these coefficients if it will be noticed that all coefficients for each $U_{n,m+j}$ must sum to unity (with the exception of the constant term which may be present). For a dozen or so sets of substitutions yielding $U_{o,m+4096}$, $U_{1,m+4096}$, etc., one may resort to a high speed computer. It was found in this problem (the one described by figure 1) that combining the difference equations in this way and using the CPC to compute the coefficients, the total overall computation time was reduced by 20 fold.

A word or two is in order concerning the boundary condition near the singularity. The solution U changes very rapidly in this neighborhood especially for the transient solution and the boundary condition (8) is not completely adequate. It was found in an early run on the CPC that the approximation (8) introduces a very nearly constant negative error into the interior of the X , t-plane. This had the effect of using a different reduced Q so that the condition:

$$\int_0^L u(z,t)\,dz \,/\, Qt = 1$$

was not fulfilled. The ratio was consistantly less than unity but essentially constant. The boundary condition (8) was used in calculating the coefficients, then when the problem itself was ready to run the boundary value $U_{o,m}$ was calculated from the condition

$$\int_0^L u(z,t)\,dz = Qt = M_0 u_{0,m} + M_1 u_{1,m} + \cdots + M_N u_{N,m}$$

i.e., the relation was solved for $U_{o,m}$. The M_i's are the weighting factors for the numerical integration. This is essentially equivalent to the differential form of the boundary conditions so it is a valid approximation. The error introduced by the numerical integration was smaller than that in the difference form of the boundary conditions (8) at X = O. Also, in this integral form the errors tended to be self correcting as the calculation proceeded. The $U_{o,m}$, $U_{1,m}$ values obtained in later runs were much higher than one would expect, but all of the rest of the points $U_{n,m}$ quickly settled down to within 3% or less of their true values as was shown when the steady state solution was reached. Even this error could be reduced by taking the mesh in the x direction finer.

This method of combining the difference equations is subject to considerable generality and applicability to other problems. It combines the higher accuracy of very fine mesh spacings (provided finer meshes provide higher accuracy to begin with) with shorter solution time found in more coarse meshes. The number of numerical operations is reduced by as much as three or four orders of magnitude for very large problems i.e., ones with difficult K(X)'s to handle, thus reducing the ever present danger of accumulated round-off error. The major limitation to this procedure is that of calculating the coefficients.

When the solution time of the given problem has been reduced to the point where it is roughly equal to the time required for the computer itself to generate the coefficients, it is felt that this is probably the point of maximum efficiency for the method.

Philip L. Phipps

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MULTI-CENTER INTEGRALS

The problem of determining multicenter integrals of atomic orbitals is still fairly difficult. The following report will review briefly the status of numerical procedures with respect to the Whirlwind computer here at M.I.T. For general references the reader should consult a recent review article by Dalgano [1].

One method of evaluating molecular integrals which is specific to two-center integrals is to limit the atomic orbitals to Slater AO's (i.e. analytic orbitals of the form $N r^{n-1} e^{-\alpha r} S_{\ell m}(\theta,\varphi)$, and then by use of prolate spheroidal coordinates express the integrations in terms of analytic functions. When this is done it is found that all one electron integrals can be simply found in terms of the two functions $A_n(X)$ and $B_n(X)$, which are only sparsely tabulated. The latter functions, however, can be generated for arbitrary arguments by means of a high-speed computer and such a generation subroutine has been written and tested [2]. (In addition, for convenience, a production-form program has been prepared for all one-electron integrals of orbitals up to 2p; computation time about 1.75 seconds per integral.) The remaining two-electron integrals fall into two groups, those with the two charge distributions each about one of the centers, (i.e. coulomb-like), and those with split charge distributions, (i.e., exchange-like). The coulomb-like integrals are also expressable in terms of the A_n and B_n functions and thus offer no great difficulty. The exchange-like integrals, however, must be evaluated by different techniques, which have been described in detail by Ruedenberg[3] of Mulliken's Group in Chicago. A Whirlwind program to evaluate these exchange-like integrals has been written by P. Merryman, also of Mulliken's Group and is currently being tested. Thus all the two-center integrals will soon be fairly easy to compute.

There are two major limitations, though, to the method just described. The first is the requirement that the orbitals be Slater AO's. For Hartree-Foch orbitals, this problem can be circumvented by fitting the function by means of a few Slater AO's [4,2]. Besides the difficulty of fitting, the only other disadvantage of this decomposition is the greatly increased number of integrals required and the consequent many numerical recombinations necessary to obtain the basic integral values. The second limitation of the above approach is the obvious inability to handle three-and four-center integrals.

A second method of calculating multicenter integrals exists which does not have these two drawbacks. This is the method of expanding all the orbitals about one of the centers. Thus if the orbitals being used are expressed in the form, $f(r_a) S_{\ell m}(\theta_a,\varphi_a)$ about center a, they can always be expanded about another center b, by virtue of the completeness of the spherical harmonics.

$$f(r_a) S_{\ell m}(\theta_a,\varphi_a) = \sum_{\ell',m'} g_{\ell' m'}(r_{ab}, r_b)\, S_{\ell' m'}(\theta_b,\varphi_b)$$

(In addition, $\frac{1}{r}$ and $\frac{1}{r_{12}}$ can be expanded in the usual series of spherical harmonics and powers of r.) Now when $f(r_a)$ is a numerically-given function, as Lowdin has shown [5], one can use straight-forward numerical procedures to find the expansion functions, $g(r_{ab}, r_b)$. When the basic orbitals are expressed in terms of Slater AO's, though, the function g is even simpler to obtain, for in this case, the g's can be written in terms of the spherical Bessel functions of imaginary argument $i_n(x)$ and $k_n(x)$. New numerical techniques have been found for easily generating these functions on a high-speed computer, and such a generation subroutine has been prepared for Whirlwind. In any case, the expansion functions, g, may be systematically prepared. Furthermore, since the multi-center integral has now been reduced to a series of one-center integrals, the integration over the angular coordinates can all be performed, a process which greatly reduces the various summations introduced by the expansions. Thus the basic integral is expressed in a series of terms each containing a radial integral which will be either of the one or two electron form:

$$\int_0^\infty r^n a(r) b(r)\, dr$$

$$\text{or} \quad \int_0^\infty a(r_1) b(r_1) \frac{dr_1}{r_1^{n+1}} \int_0^{r_1} r_2^n c(r_2) d(r_2)\, dr_2$$

where a, b, c, and d are, in general, numerically given functions about one of the centers. Because, in a complete calculation one may require several hundred of these integrals, a Whirlwind program for doing these numerical quadratures has been written and tested. In the interest of program speed, Simpson's rule is used for the integrations, but the mesh size can be essentially arbitrarily small and with as many scale doublings as desired. To give a very rough notion of the computation time required, a basic 2-outer exchange integral might involve a series of about six significant terms, each of which requires about five seconds to compute, giving a total time which compares well with even the explicit two-center method.

Thus the method of expanding all functions about one-center appears very attractive for the three and four-center integrals. The writer plans to use this method to evaluate the more important three-center integrals occurring in a tight-binding calculation of Graphite.

F. J. Corbató

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EIGEN VALUES FOR A SPHEROIDAL SQUARE WELL

I. For conciseness the description of the problem will be restricted to the case of the oblate spheroid [1]. We define the co-ordinates μ, η, φ which are defined in the regions $\left\{ \begin{array}{l} 0 \le \mu \le \infty \\ -1 \le \eta \le 1 \\ 0 \le \varphi \le 2\pi \end{array} \right\}$ The problem is to find the eigen values of the time-independent Schroedinger equation

$$(1) \qquad [\nabla^2 + k^2 - V(\mu)]\,\psi(\eta, \mu, \varphi) = 0$$

where V is a step function

$$V(\mu) = 0 \;, \quad \mu < a$$
$$\quad = V_0 \;, \quad \mu > a \,.$$

Now if d is the focal distance for the spheroid, and if one defines

$$h^2 = d^2\, k^2 ; \; g^2 = d^2\, (k^2 - V_0)$$

then the solutions inside and outside the spheroid, respectively may be written

$$(2a) \qquad \psi_i = \sum_\ell a_\ell^m S_{m\ell}(h, \eta)\, je_{m\ell}(h, \mu)\, e^{im\varphi} \;, \quad \mu < a$$

$$(2b) \qquad \psi_o = \sum_\lambda b_\lambda^m S_{m\ell}(g, \eta)\, he_{m\lambda}(g, \mu)\, e^{im\varphi} \;, \quad \mu > a \,.$$

The a_ℓ^m and b_λ^m are constants (to be determined) and the $S_{m\ell}, je_{m\ell}, he_{m\ell}$ functions are as defined in Morse and Feshbach.

In order that the ψ which is of the form (2a) for $\mu < a$ and of form (2b) for $\mu > a$ be a solution of (1) at $\mu = a$, it is necessary that

$$(3) \qquad [\psi_i - \psi_o]_{\mu = a} = 0$$

$$\left[\frac{\partial}{\partial\mu}(\psi_i - \psi_o)\right]_{\mu = a} = 0.$$

Defining the function of g and h

$$C_{\lambda\ell} = [\Lambda_{m\lambda}(g)]^{-1} \int_{-1}^{1} S_{m\lambda}(g, \eta)\, S_{m\ell}(h, \eta)\, d\eta$$

where

$$\int_{-1}^{1} S_{m\lambda}(g, \eta)\, S_{m\nu}(g, \eta)\, d\eta = \Lambda_{m\lambda}\, \delta_{\lambda\nu} \,,$$

the equations (3) lead to the matrix equation

$$(4) \qquad A \cdot \vec{a} = 0$$

where $\vec{a}$ is a vector with components a_ℓ and A is an infinite square matrix with elements

$$A_{\lambda\ell} = C_{\lambda\ell} \left\{ je_{m\ell}(h, \mu) \frac{d}{d\mu} \ln \frac{je_{m\ell}(h, \mu)}{he_{m\ell}(g, \mu)} \right\}_{\mu = a} \cdot \qquad (h^2 - g^2) = d^2 V_0$$

In the usual way it is seen that a non-trivial solution of equation (4) may be found by requiring that

$$\det A = 0$$

and the values of $k^2 = h^2/d^2$ for which this determinental equation is true are the eigen values of equation (1).

If one chooses to think of the $C_{\lambda\ell}$ in terms of their role as expansion coefficients, i.e.

$$S_{m\ell}(h, \eta) = \sum_\lambda \frac{1}{\Lambda_{m\lambda}} C_{\lambda\ell}\, S_{m\lambda}(g, \eta)$$

it is immediately obvious that in general the expansion on the right cannot be expected to terminate. For if it did we could set g = o (so that $S_{m\ell}$ would become the associated Legendre polynomical P_ℓ^m) and obtain a finite relationship between $S_{m\ell}(h, \eta)$ and the P_ℓ^m. But such a relationship does not exist.[1]

On the other hand the differential equation for $S_{m\ell}$ which is

$$\left\{ \frac{d}{d\eta}(1 - \eta^2)\frac{d}{d\eta} + A_{m\ell} - \frac{m^2}{1 - \eta^2} - h^2\eta^2 \right\} S_{m\ell} = 0$$

indicates that (since $A_{m\ell}$ is a monotonic increasing function of ℓ)[2] that for $A_{m\ell} >> h^2$ the differential equation should approach the equation for $P_\ell^m(\eta)$. Thus, for large ℓ and λ the coefficients $C_{\ell\lambda} \to 0$ $(\ell \neq \lambda)$. For $\ell >> \lambda$ (or vice-versa) the same argument would indicate that

$$C_{\ell\lambda} \to d_\ell(g \,|\, m\lambda) \qquad \text{where by definition}$$

$$S_{m\ell} = \sum_{n=0}^{\infty} d_n(g \,|\, m\lambda)\, P_{m+n}(\eta) \,.$$

But it is known that

$$d_n \xrightarrow[n \to \infty]{} g^2/\eta^2$$

so that in the worst case the off-diagonal elements appear to converge roughly as $1/\ell^2$.

The preceding argument shows in a rather qualitative fashion that the determinant is likely to be convergent. A more rigorous argument which will also discuss the behavior of the diagonal elements will be given in a later report.

II. It seems likely that it will be necessary to compute a large number of spheroidal functions in order to solve the problem outlined in the previous section. In order to do this I plan to use the Whirlwind program previously developed and reported upon by F. Corbato and J. D. C. Little.[3] However, Mr. Corbato has found that his program in its original form could not be used for values of h much in excess of h=8. For values of h much in excess of this value the iterative process used in the original program becomes extremely sensitive to the initial guess (for the eigen value), and if this guess is not sufficiently accurate the process will converge to the wrong eigen value. In order to improve the initial guess we (Mr. Corbato and myself) are computing the eigen value directly by means of an asymptotic formula.[4]

Preliminary runs seem to indicate that the asymptotic formula gives a surprisingly good estimate of the eigen value for values of h as low as 5. If this behavior is consistent it may reduce the average time needed to compute spheroidal wave functions by as much as 30%.

Jack L. Uretsky

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VARIATIONAL DETERMINATION OF ATOMIC WAVE FUNCTIONS

During the past quarter, most of the time has been spent programming for Whirlwind. The variational calculations for the three parameter wave functions of Morse, Young, and Haurwitz. [1]

The actual evaluation of the energy for any particular set of parameters is very easy to program. There are two basic integrals, the first being the rather trivial function

$$(1) \qquad A_n(\alpha) = \int_0^\infty e^{-\alpha r} r^n\, dr = n!/\alpha^{n+1}$$

involved in the matrix elements for the kinetic and nuclear potential energies. The second one is involved in the electronic repulsion and exchange terms.

$$I_{n\,q\alpha}^{\,p\beta} = \int r_1^{\,p} e^{-\beta r_1} P_n^m(\cos\varphi_1)\, \frac{2}{r_{12}}\, r_2^{\,q} e^{-\alpha r_2} P_n^m(\cos\varphi_2)\, dr_1\, dr_2$$

$$= \frac{32\,\pi^2}{(2n+1)^2}\left[\frac{(n+|m|)!}{(n-|m|)!}\right] S_\alpha^\beta(p,q,n) \qquad (2)$$

The function $S_\alpha^\beta(p,q,n)$ is discussed in Quarterly Progress Report No. 9, September 15, 1953. In general, it can be written as

$$S_\alpha^\beta(p,q,n) = \left(\sum_{r=0}^{N} a_r x^{r+S_1}\right) / \alpha^2(\alpha+\beta)^{S_2}, \quad x = \alpha/\beta .$$

S_1 and S_2 are integers and along with the a_r are functions of p, q, and n.

The central problem has been to obtain, using the shortest possible amount of machine time, the energy minimum correct to three decimal places.

The first minimization scheme tried was a second order Lagrangian interpolation. It proved to be highly inefficient, a large number of points over a small region being required for a reasonably accurate extremum.

During the past three weeks, a new approach has been tried. The technique, commonly referred to as the method of steepest descent, may be summarized as follows. An initial guess of the parameters (a_o, b_o, c_o) is made and the valve of the energy and the partial derivatives $\frac{\partial W}{\partial a}, \frac{\partial W}{\partial b}, \frac{\partial W}{\partial c}$ are determined. From the latter we obtain the gradient vector whose negative direction is along the path for which the energy decreases most rapidly. Since we are looking for a minimum, we take the next point along a line parallel to the gradient vector. By properly scaling the distances between successive points, we should be able to converge to the minimum.

For the actual machine computation, we first estimate the maximum distance of our initial point from the minimum. Let this be called Δ_o. The next point is then chosen to be

$$a_1 = a_o - \Delta_o \cos\varphi_a$$

$$b_1 = b_o - \Delta_o \cos\varphi_b$$

$$c_1 = c_o - \Delta_o \cos\varphi_c$$

where $\cos\varphi_a$,etc. are the direction cosines of the gradient. After that four more points are calculated, the distance between successive points being scaled by a factor of two each time. Such a procedure should give an extreme point with the maximum uncertainties in the parameters given by

$$(\Delta a)_{max} \approx \Delta_o (\cos\varphi_a)_{min} / 16$$

$$(\Delta b)_{max} \approx \Delta_o (\cos\varphi_b)_{min} / 16$$

$$(\Delta c)_{max} \approx \Delta_o (\cos\varphi_c)_{min} / 16$$

where the direction cosines are evaluated at the point of minimum calculated value.

The partial derivatives are calculated by taking first differences of W for parameter increments of o.o1.

By using the generalized concepts of distance, gradient, etc. in N dimensional cartesian space, we may extend the preceding argument to the case of functions of any number of parameters.

The method has been tried for the ground state $(1S^2\ 2S^2\ 2P)\ ^2P$ of Boron, and the results appear to be correct to one unit in the third decimal place. Several further checks are being made by starting at different points and using different values for Δ_o. If the results are satisfactory, a systematic program for calculating the energies of the states not yet computed in previous hand and IBM calculations will be set up.

The possibility of adding a 3S function to the present scheme is now being investigated by two seniors Robert Papa and Alfred Finn who are doing a joint B.S. thesis in the Physics Department on the calculation of the ground state of sodium and several other states involving a 3S orbital. They are working with a three parameter form for the 3S function with the hope that they might deduce a rule for fixing one or two of the parameters.

Finally, programs for calculating the configuration interaction integrals involved in the pertubation correction terms[2] are being written for substitutions involving 3s, 3p, and 3d orbitals.

Arnold Tubis

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NEUTRON-DEUTERON SCATTERING

The variational calculation of S-state phase shifts in neutron-deuteron scattering is nearing completion. We indicate here an outline of the theory.

Assuming two-body central forces of arbitrary exchange character, the Schrodinger equation for a system of three particles of equal mass takes the form

$$\left[\nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \frac{2m}{\hbar^2}(E - V)\right]\Psi = 0 \qquad (1)$$

where

$$V = V_{12} + V_{13} + V_{23}$$

$$V_{ij} = U_{ij}\,(w + m\,M_{ij} + b\,B_{ij} + h\,M_{ij}\,B_{ij}) \qquad (2)$$

M_{ij} and B_{ij} being the operators which exchange the space and spin coordinates, respectively, of particles i and j. U_{ij} is a scalar function of the distance r_{ij} and w, m, b, h are numerical coefficients whose sum is unity.

After the motion of the center of mass is separated off, there remain six coordinates to describe the system. For the scattering problem in question the appropriate choice is that of the vectors $\vec{r}$ and $\vec{q}$, where $\vec{r}$ is proportional to the deuteron coordinate and $\vec{q}$ is the vector from the incident neutron to the center of mass of the deuteron. (Fig. 1; it is assumed that particles 2 and 3 form the original deuteron pair). It can be seen that the magnitudes r and q, together with α, the angle between the two vectors, are sufficient to

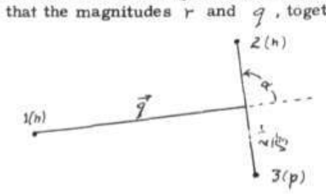

Fig. 1

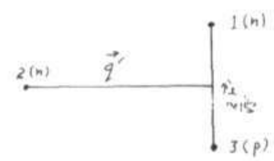

Fig. 2

determine the relative position of the three particles in their plane. The remaining three coordinates then describe the orientation of this plane. For low energy (S-state) scattering, the wave function will be independent of this orientation and will thus be a function only of r, q and α. These coordinates are of course expressible in terms of the interparticle distances, which furnish an analogous specification of the relative location of three particles in their plane. The relations are:

(3a) $$r = \frac{\sqrt{3}}{2} r_{23}$$

(3b) $$q = \tfrac{1}{2} \sqrt{\{2(r_{12}^2 + r_{13}^2) - r_{23}^2\}}$$

(3c) $$\cos\alpha = (r_{12}^2 - r_{13}^2) / r_{23} \sqrt{\{2(r_{12}^2 + r_{13}^2) - r_{23}^2\}}.$$

Instead of α, we shall eventually use as a third coordinate the distance S, the third side of the triangle formed by $\vec{r}$ and $\vec{q}$. This is given by

(3d) $$S = \sqrt{(r^2 + q^2 - 2rq\cos\alpha)} = \sqrt{\left(\tfrac{1}{2} r_{23}^2 + \left(\tfrac{1-\sqrt{3}}{2}\right) r_{12}^2 + \left(\tfrac{1+\sqrt{3}}{2}\right) r_{13}^2\right)}.$$

We also find it necessary to define the coordinates $\vec{r}'$, $\vec{q}'$ the result of M_{12} (neutron exchange) operating on the original $\vec{r}$ and $\vec{q}$. (Fig. 2) r', q' and S' are expressible as quadratic forms in r, q and S.

(4a) $$r' = \tfrac{1}{2}\sqrt{\left(q^2(3-\sqrt{3}) + r^2(1-\sqrt{3}) + \sqrt{3}\,S^2\right)}$$

(4b) $$q' = \tfrac{1}{2}\sqrt{\left(q^2(1+\sqrt{3}) + r^2(3+\sqrt{3}) - \sqrt{3}\,S^2\right)}$$

(4c) $$S' = \sqrt{\left(q^2\left(\tfrac{1-\sqrt{3}}{2}\right) + r^2\left(\tfrac{1+\sqrt{3}}{2}\right) + \tfrac{1}{2}S^2\right)}$$

Writing equation (1) in the $\vec{r}$, $\vec{q}$ system and expanding in partial waves, we have for the S-wave part of the resulting equation:

(5) $$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{\partial \Psi}{\partial r}\right) + \frac{1}{q^2}\frac{\partial}{\partial q}\left(\frac{\partial \Psi}{\partial q}\right) + \left(\frac{1}{r^2} + \frac{1}{q^2}\right)\frac{1}{\sin\alpha}\frac{\partial}{\partial\alpha}\left(\sin\alpha\frac{\partial\Psi}{\partial\alpha}\right) + \frac{4m}{3\hbar^2}(E_k - E_d - V)\Psi = 0$$

where E_K is the kinetic energy of the incident neutron in the center of mass system (= $\frac{2}{3}$ the energy in the lab system) and E_d is the binding energy of the deuteron.

The wave function Ψ in (5) is a combination of spatial and spin functions, and must be antisymmetric in the two neutrons to satisfy the Pauli principle.[1] We therefore write explicitly, for the quartet and doublet spin states (S = 3/2, 1/2 respectively):

(6a) $$\Psi_Q = \chi_Q(\psi_Q - \psi_Q')$$

(6b) $$\Psi_D = \chi_{D1}(\psi_D - \psi_D') + \chi_{D2}(\psi_D + \psi_D')$$

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[1] We do not utilize the isotopic spin formalism, as we find it more convenient to label each particle explicity as neutron or proton.

Here ψ_Q is the (totally symmetric) quartet spin function; and is therefore multiplied by a spatial function antisymmetric in the neutrons ($\psi' = M_{12}\psi$). In the doublet state there are two independent spin functions (for each value of m_S). We choose χ_{D1} to be the one symmetric in the neutrons and χ_{D2} the one antisymmetric, and multiply each by the appropriate space function so as to antisymmetrize the total wave function. We now put (6a) and (6b) into (5), introduce the notation $\psi = \frac{u}{rq}$ and sum over spin coordinates. The resulting equation for the quartet scattering is:

(7) $$\left[T + \frac{k^2 - k_d^2}{rq}\right](u - \bar{u}) + rq\,\Omega\,(u - \bar{u})/rq = 0$$

where we have introduced the following additional notation:

(8) $$T \equiv \frac{1}{rq}\left[\frac{\partial^2}{\partial r^2} + \frac{\partial^2}{\partial q^2} + \left(\frac{1}{r^2} + \frac{1}{q^2}\right)\left(\frac{\partial^2}{\partial\alpha^2} + \cot\alpha\frac{\partial}{\partial\alpha}\right)\right]$$

(9) $$\bar{u} \equiv \frac{rq}{r'q'} M_{12}\,u$$

(10a) $$k^2 = \frac{4m}{3\hbar^2} E_k$$

(10b) $$k_d^2 = \frac{4m}{3\hbar^2} E_d$$

(10c) $$\Omega = -\frac{4m}{3\hbar^2} V$$

For the doublet scattering we obtain instead of (7) the two equations

(11a) $$\left[T + \frac{k^2 - k_d^2}{rq}\right](u - \bar{u}) + rq\left[\Omega_{aa}\frac{(u-\bar{u})}{rq} + \Omega_{ab}\frac{(u+\bar{u})}{rq}\right] = 0$$

(11b) $$\left[T + \frac{k^2 - k_d^2}{rq}\right](u + \bar{u}) + rq\left[\Omega_{ba}\frac{(u-\bar{u})}{rq} + \Omega_{bb}\frac{(u+\bar{u})}{rq}\right] = 0$$

where

(12a) $$\Omega_{aa} = U_{12}[w + b + (m+h)M_{12}] + U_{13}\left[\left(w - \tfrac{b}{2}\right) + \left(m - \tfrac{h}{2}\right)M_{13}\right] + U_{23}\left[\left(w - \tfrac{b}{2}\right) + \left(m - \tfrac{h}{2}\right)M_{23}\right].$$

(12b) $$\Omega_{ab} = \Omega_{ba} = U_{13}\left[\tfrac{\sqrt{3}}{2}(b + hM_{13})\right] + U_{23}\left[-\tfrac{\sqrt{3}}{2}(b + hM_{23})\right]$$

(12c) $$\Omega_{bb} = U_{12}[w - b + (m-h)M_{12}] + U_{13}\left[\left(w + \tfrac{b}{2}\right) + \left(m + \tfrac{h}{2}\right)M_{13}\right] + U_{23}\left[\left(w + \tfrac{b}{2}\right) + \left(m + \tfrac{h}{2}\right)M_{23}\right]$$

We shall proceed with the derivation of the quartet scattering. The doublet gives longer equations, but proceeds analogously.

The boundary conditions on Ψ and u are the following:

a) Ψ must be everywhere finite; hence $u = 0$ when either $r = 0$ or $q = 0$.

(13) b) when $q \to \infty$, $\psi \to F(r)\sin(kq + \delta)/q \sin\delta$

where F (r) is the deuteron ground state wave function, and δ is the phase shift which describes the scattering. Hence we have, for $q \to \infty,\ r < \infty$,

(14) $$u \to rF(r)\sin(kq+\delta)/\sin\delta \equiv W = W_1 + W_2\cot\delta$$

(15a) where $$W_1 = rF(r)\cos(kq)$$

(15b) $$W_2 = rF(r)\sin(kq).$$

W_1 and W_2, and hence W, the asymptotic form of u, satisfy the equation

(16a)
(16b) $$\left[T + \frac{k^2 - k_d^2}{rq}\right]\begin{Bmatrix} W \\ W_1 \\ W_2 \end{Bmatrix} + rq\,\Omega_{23}\begin{Bmatrix} W \\ W_1 \\ W_2 \end{Bmatrix}\frac{1}{rq} = 0$$
(16c)

Together with (13) and (14), we have the boundary condition for exchange scattering, $q' \to \infty,\ r' < \infty$,

(17a) $$\psi' \to F(r')\sin(kq'+\delta)/q'\sin\delta$$

(17b) $$\bar{u} \to \frac{rq}{q'}F(r')\sin(kq'+\delta)/\sin\delta \equiv \bar{W} = \bar{W}_1 + \bar{W}_2\cot\delta$$

where now F(r') is the deuteron function in the exchange coordinates, and W_1 and W_2 are given by

(18a) $$\bar{W}_1 = \frac{rq}{q'}F(r')\cos(kq')$$

(18b) $$\bar{W}_2 = \frac{rq}{q'}F(r')\sin(kq')$$

$\bar{W}$, $\bar{W}_1$ and $\bar{W}_2$ are solutions of

(19a)
(19b) $$\left[T + \frac{k^2 - k_d^2}{rq}\right]\begin{Bmatrix} \bar{W} \\ \bar{W}_1 \\ \bar{W}_2 \end{Bmatrix} + rq\,\Omega_{13}\begin{Bmatrix} \bar{W} \\ \bar{W}_1 \\ \bar{W}_2 \end{Bmatrix} = 0$$
(19c)

The actual boundary conditions are of course on the total wave function of the system, which is $\psi - \psi'$. However it is impossible for both ψ and ψ' to contribute at infinity, since they go to deuteron functions in different coordinates (r and r'). That is, if one neutron is at infinity then either r or r' must be infinite and the deuteron function, which drops off exponentially will kill the contribution of that part. This means that ψ is used to satisfy the boundary condition for ordinary scattering and ψ' (or $\bar{u}$) for exchange scattering.

At this point we introduce the inside wave functions χ, $\bar{\chi}$, defined by

(20a) $$\chi = w - u$$
(20b) $$\bar{\chi} = \bar{w} - \bar{u}$$

From (7), (16) and (19) we obtain the differential equation for $\chi - \bar{\chi}$,

(21) $$\left[T + \frac{k^2 - k_d^2}{rq}\right](\chi - \bar{\chi}) + rq\left\{V(\chi - w - \bar{\chi} + \bar{w})/rq + V_{23}\frac{w}{rq} - V_{13}\frac{\bar{w}}{rq}\right\} = 0$$

The boundary conditions on χ are

(22a) $$\chi(q=0) = rF(r)$$
(22b) $$\chi(r=0) = 0$$
(22c) $$\chi(q=\infty) = 0$$
(22d) $$\chi(r=\infty) = 0$$

Starting from equation (21) many variational principles for the phase shift δ can be constructed, as pointed out by Rubinow [1] for the two-body problem.

The general procedure is as follows: from (21) (16a) and (19a) we write the differential equation for $(\chi - w_1 - \bar{\chi} + \bar{w}_1)$:

(23) $$\left[T + \frac{k^2 - k_d^2}{rq}\right](\chi - \bar{\chi} - w_1 + \bar{w}_1) + rq\{\Omega(\chi - w_1 - \bar{\chi} + \bar{w}_1)/rq - \cot\delta\,[\Omega(w_2 - \bar{w}_2)/rq - \Omega_{23}w_2/rq + \Omega_{13}\bar{w}_2/rq]\}$$

Multiplying this equation by $\frac{(\chi - w_1 - \bar{\chi} + \bar{w})}{rq}$, (16a)-(19a) by $\frac{(2\chi - w_1 - 2\bar{\chi} + \bar{w}_1)}{rq}$, adding and integrating over all space ($d\tau = r^2q^2\,dr\,dq\,\sin\alpha\,d\alpha$) we obtain, after a partial integration of the second derivatives,

(24) $$B(k\cot\delta) = C + L_2$$

where

(25a) $$B = \frac{1}{k}\int_0^\infty dr\int_0^\infty dq\int_0^\pi \sin\alpha\,d\alpha\; rq\left\{(\chi - w_1 - \bar{\chi} + \bar{w}_1)\left[(\Omega - \Omega_{23})\frac{w_2}{rq} - (\Omega - \Omega_{13})\frac{\bar{w}_2}{rq}\right]\right\}$$

$$C = \int_0^\infty dr\int_0^\infty dq\int_0^\pi \sin\alpha\,d\alpha\left\{-\left[\frac{\partial}{\partial r}(\chi - \bar{\chi})\right]^2 - \left[\frac{\partial}{\partial q}(\chi - \bar{\chi})\right]^2 - \left(\frac{1}{r^2} + \frac{1}{q^2}\right)\left[\frac{\partial}{\partial\alpha}(\chi - \bar{\chi})\right]^2\right.$$

(25b) $$\left. + (k^2 - k_d^2)(\chi - \bar{\chi})^2 + rq\left\langle(\chi - w_1 - \bar{\chi} + \bar{w}_1)\,\Omega\left(\frac{\chi - w_1 - \bar{\chi} + \bar{w}_1}{rq}\right) + (2\chi - w_1 - 2\bar{\chi} + \bar{w}_1)\left(V_{23}\frac{w_1}{rq} - V_{13}\frac{\bar{w}_1}{rq}\right)\right\rangle\right\}$$

$$L_2 = \int_0^\infty dr\int_0^\pi d\alpha\,\sin\alpha\left\{\left[(\chi - \bar{\chi} - w_1 + \bar{w}_1)\frac{\partial}{\partial q}(\chi - \bar{\chi}) + (\chi - \bar{\chi})\frac{\partial}{\partial q}(w_1 - \bar{w}_1)\right]_{q=0}^{q=\infty}\right\}$$

(25c) + similar derivatives in r and α

Again, on multiplying (23) by ($W_2 - \bar{W}_2$), (16b)-(19b) by ($\chi - w_1 - \bar{\chi} + \bar{w}_1$), subtracting and integrating we obtain

(26) $$B + L_1 = A\,k\cot\delta$$

where

(27a) $$A = \frac{1}{k^2}\int_0^\infty dr\int_0^\infty dq\int_0^\pi \sin\alpha\,d\alpha\; rq\left\{(w_2 - \bar{w}_2)\left[(\Omega - \Omega_{23})w_2/rq - (V - V_{13})\bar{w}_2/rq\right]\right\}$$

(27b) $$L_1 = \int_0^\infty dr\int_0^\pi \sin\alpha\,d\alpha\left\{\left[(w_2 - \bar{w}_2)\frac{\partial}{\partial q}(\chi - \bar{\chi}) - (\chi - \bar{\chi})\frac{\partial}{\partial q}(w_2 - \bar{w}_2)\right]_{q=0}^{\infty}\right\}$$

+ similar derivatives in r and α .

L_1 and L_2 are determined from the boundary conditions, and do not depend on the nature of χ . Neither equation (24) nor (26) is stationary, but suitable combinations may be taken which will have the desired property of stationarity. The simplest of these combinations is obtained by rewriting (24) as

(28) $$(B + L_1)\,k\cot\delta = C + L_2 + L_1(k\cot\delta)$$

Substituting for $k \cot \delta$ from (26) we obtain

$$(29) \quad k \cot \delta = \frac{1}{L_1} \left[(B + L_1)^2 / A - (C + L_2) \right]$$

It may be verified that (29) is stationary with respect to variations in ψ and $\bar{\psi}$ which satisfy the boundary conditions (22). The problem now consists of choosing a suitable trial function ψ, dependent on a number of variational parameters, and "minimizing" with respect to the parameters. Since we are dealing with phases, which are not positive definite, it is not known a priori whether the stationary point will be a maximum, minimum, or a point of inflection.

The integrals which appear in expressions (25) and (27) are in general extremely complicated, mainly as a result of the exchange operators and the mixture of primed and unprimed coordinates. Any function linear in one set of coordinates is a sum of radicals in the other set, and the exchange operators introduce various sets of such radicals. The best chance of obtaining a reasonable solution lies in the use of Gaussian forms for both the potentials and the trial functions, since linear forms in the squares of one set of coordinates will again be linear in the other set. Accordingly we choose for the spatial dependence of the two-body potentials,

$$(30) \quad V_{ij} = V_o \exp \left[- r_{ij}^{\,2} \right]$$

where we have taken the range of the force as our unit of length. (All the calculations are performed in dimensionless form). The depth V_o is a compromise between the values required to find the deuteron and the triton correctly; in the absence of tensor forces especially, these two data are at variance: a well deep enough to give the correct binding energy of the deuteron gives too much binding for the triton. The values of the constants w, m, b, h in (2) are left arbitrary, except that the singlet-triplet ratio in the 2 body S state gives a constraining relation

$$(31) \quad w + m - b - h = 1 - 2g \approx .6$$

For our trial function we take

$$(32) \quad \psi = r \exp \left[-\lambda r^2 - b q^2 - \mu s^2 \right]$$

which satisfies the boundary conditions provided $\lambda + \mu$ is a constant determined by the deuteron wave function. We therefore have essentially a two-parameter trial function . Putting $\mu = o$ corresponds to the no polarization assumption, i.e. assuming that the wave function is everywhere a deuteron function in one pair of coordinates multiplied only by a function of g. This assumption has been made in all previous calculations of the problem.[2,3,4] The size of the "best" value of μ, as well as the effect on the actual phase shifts, will be a measure of the importance of polarization in the low-energy scattering.

If we expand equation (29) in powers of k^2, then the zero order term will be the negative reciprocal scattering length, as usually defined, and the coefficient of k^2 will be half the effective range. These are quantities which can be compared with experiment. The expansion is effected by performing an analogous expansion for each of the quantities A, B, C, L_1, L_2 appearing in (24) and (26).

With the trial function (32), all the integrals are tractable, using methods which will be discussed in a future report. The integrations are first transformed to (r, q, s) space in which the volume element is r q s dr d q d s, and in which the limits on the s integration go from $|r-q|$ to $r+q$. The integrals which give the most difficulty are these arising from the "crossed" derivatives in (25b), e.g. $\frac{\partial \psi}{\partial q} \frac{\partial \bar{\psi}}{\partial q}$. A small number of these can only be reduced to one dimensional integrals which must then be performed numerically. The remainder are all integrated exactly.

The calculation of the quartet scattering length has been programmed for the Whirlwind Computer, using CS II, and trouble shooting has been successfully completed. (Results for a trial point have been checked by a hand computation). The calculation of the variational expression (29) for one value of the variational parameters,takes 45 seconds of machine time, a considerable amount. We must therefore be comewhat frugal in our search for the stationary point, and possible methods of systematic search are being considered. The search is complicated

by the fact, previously mentioned, that we do not know whether we are looking for a true minimum or a saddle point. The plot of $k \cot \delta$ versus b for $\mu = o$ (no polarization) shows a fairly sharp minimum, corresponding to a positive scattering length of reasonable magnitude. However, preliminary calculations show that the integrals are extremely sensitive to the value of μ, and lead one to suspect that the desired stationarity is quite likely to be a saddle point.

Leo Sartori

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NUCLEAR CONSTITUTION

Some headway has been made in determining the importance of the exchange potential which arises in a Hartree-Foch calculation for a nucleus.

The Hartree-Foch equations are

$$(K.E.) \; \psi_i(r) + \Big(\sum_j \int \psi_j^*(r') V(r-r') \psi_j(r') \, dr' \Big) \psi_i(r) - \Big(\sum_j \int \psi_j^*(r') V(r-r') \psi_i(r') \, dr' \Big) \psi_j(r) = E_i \psi_i(r).$$

$V(r-r')$ is the internuclear potential.

It is the third term in this equation which is awkward because it is not in operator form and it changes for each particle. The nucleus we are working with has 184 particles, so the solution of the HF equations would present quite a formidable task.

Fortunately, the third term can be put into operator form and averaged over all particles, so each particle seems to be traveling in the same effective potential, or 'pot'. The equations then take the form

$$\Big[K.E. + \sum_j \int \psi_j^*(r') V(r-r') \psi_j(r') \, dr' - \sum_{k,j} \int \psi_j^*(r') \psi_k(r) V(r-r') \psi_j^*(r) \psi_k(r') \, dr' \Big/ \sum_j |\psi_j(r)|^2 \Big] \psi_i(r) = E_i \psi_i(r).$$

It is obvious now that the pot is formedby the last two terms on the left, the classical and the exchange potential.

The integrations have been carried out for $V(r-r') = V_o e^{-\alpha r^2}$ and spherical square-well eigenfunctions for the ψ's. It has been found that the exchange potential is about 15% of the depth of the classical potential. The shape of the two is similar, the tail of the total pot being about the same as the tail of the internuclear potential. This last remark was verified by carrying out a calculation using a Yukawa interaction which has a long tail compared to the Gaussian interaction.

It is to be noted that there is nothing self-consistent about the calculations so far. The next step is to find the best harmonic-oscillator wave functions by using the variational principle. The nucleus will, of course, collapse. To prevent collapse, Majorana forces will be added to the internucleon potential: $V = V_1 (1 + \xi P(r r'))$. $P(r r')$ exchanges r and r' i.e., attracts for symmetric and repels for antisymmetric states, and ξ is the strength of the exchange force. ξ will be varied until the binding energy of the last particle in the 'pot' is the same as it was in the square well.

M. Rotenberg

COULOMB WAVE FUNCTIONS

The irregular solution together with the derivatives of both and regular and irregular solutions has been successfully programmed. via the integral representation. It will be recalled that the Coulomb Wave Functions are given by:

$$F_L = C_L(\eta)\rho^{L+1}\Phi_L(\eta,\rho)$$

$$G_L = C_L(\eta)\rho^{L+1}g_L(\eta,\rho)$$

$$F_L' = \frac{\partial F_L}{\partial \rho} = C_L(\eta)\{(L+1)\rho^L\Phi_L + \rho^{L+1}\Phi_L'\}$$

$$G_L' = C_L(\eta)\{(L+1)\rho^L g_L + \rho^{L+1}g_L'\}$$

the integrals being

$$\Phi_L(\eta,\rho) = \int_0^\infty \cos[\rho \tanh\xi - 2\eta\xi]/[\cosh\xi]^{2L+2}\,d\xi$$

$$g_L(\eta,\rho) = \int_0^\infty\{(1+\xi^2)^L e^{-\rho\xi + 2\eta\tan^{-1}\xi} - \sin[\rho\tanh\xi - 2\eta\xi]/[\cosh\xi]^{2L+2}\}\,d\xi$$

The only essentially new integral is the one

$$\int d\xi\,(1-\xi^2)^L e^{-\rho\xi + 2\eta\tan^{-1}\xi}$$

Everything else being done by a simple modification of the program for $\Phi_L(\eta,\rho)$.

The above integral is evaluated by a seven point interpolation scheme. with a mesh size of 0.1. When the integrand becomes smaller than $(10)^{-6}$ the integration is cut off. In evaluating the intergrand, we first calculate the quantity

$$(1+\xi^2)e^{\frac{1}{L}[-\rho\xi + 2\eta\tan^{-1}\xi]}$$

and the raise it to the Lth power. This procedure eliminates the possibility that the factor $(1+\xi^2)^2$ if evaluated by itself might become too large for the machine to handle.

Some results are as follows. From our program, for the set of values $L=0,\ \rho=1,\ \eta=2$

we get:

$$F_L = +2.889590\,(10)^{-2}$$
$$F_L' = +6.130964\,(10)^{-2}$$
$$G_L = +9.800340$$
$$G_L' = -1.381263\,(10)^{-1}$$
$$F_L'\,G_L - G_L'\,F_L = +9.959840\,(10)^{-1}$$

From the National Bureau of Standards Tables

$$F_L = +2.889859\,(10)^{-2}$$
$$F_L' = +6.131009\,(10)^{-2}$$
$$G_L = +9.800520$$
$$G_L' = -1.381230\,(10)^{-1}$$
$$F_L'\,G_L - G_L'\,F_L = +1.000027$$

At present we are trying to improve the accuracy by making more use of buffers and adjusting the mesh size.

Aaron Temkin
Arnold Tubis

COMPUTATION OF CHEMICAL ENGINEERING PROBLEMS OF MULTISTAGE DISTILLATION, ABSORPTION, AND EXTRACTION

The last quarterly period has been devoted primarily to interpretation and presentation of results obtained earlier by machine computation on Whirlwind I. No new machine programs have been developed. A few additional results have been obtained, largely to refine some details.

It is concluded that this approach is very worthwhile for study of problems in this area, particularly those dealing with unsteady-state operations. A substantial number of qualitative and quantitative conclusions have been obtained. Some of these have been discussed in preceding reports. It is expected that there will be published in the near future. Consequently they will not be discussed further at this time. There are still a substantial number of unsolved problems in this field however. It is recommended that further work be done on them using this method of approach.

John F. O'Donnell

RESPONSE OF A FIVE-STORY FRAME BUILDING TO DYNAMIC LOADING

Work has been completed on a new program which should more nearly represent the behavior of this building. Our original program assumed infinitely stiff girders and thus the formation of all plastic hinges was limited to the columns. A hand analysis which is now available indicates that the girders in this particular type of structure are relatively weak and thus permit the formation of plastic hinges. Our new procedure allows for some plastic action in the girders and also computes the column resistances in each story as a function of all five floor deflections instead of limiting the influence to the two adjacent floor deflections.

Our original program has been used for four loading conditions which will be checked with the modified program. The two programs will then be used to compute the response of the structure for about 25 more loadings which are now being calculated. By using both programs we hope to be able to investigate the effect on the structure of plastic hinge formation in the girders. A number of hand solutions will be carried out to check our results.

Charles W. Johnson

ANALYSIS OF A TWO STORY STEEL FRAME BUILDING UNDER DYNAMIC LOADING

The upper story of the two story steel frame building is connected to the lower story by both columns and diagonals while the lower story is supported by columns only. We are interested in determining the dynamic load which will cause a specified deflection and thus result in the collapse of the structure. We also want to find the effect on the values of the critical load of varying the resistance characteristics.

The building is approximated by a two mass system as shown below

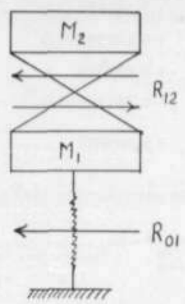


FIG. 1

The upper and lower masses are connected by a plastic resistance R_{12} which prevents relative movements between the two masses until $(R_{12})_{max.}$ is reached (see below).

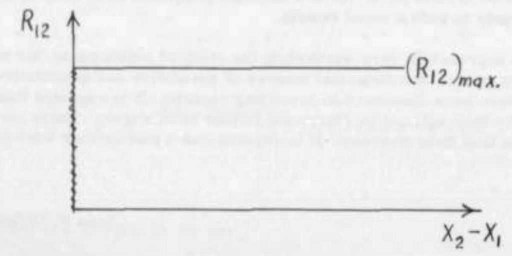


FIG. 2

Thereafter $(R_{12})_{max.}$ is considered to be the resistance to relative motion. The lower mass is supported by a spring which supplies a resistance proportional to the deflection of the lower mass but the resistance must be less than $(R_{01})_{max.}$ $[\,R_{01} \sim X_1\,,\ R_{01} \leq (R_{01})_{max.}\,]$

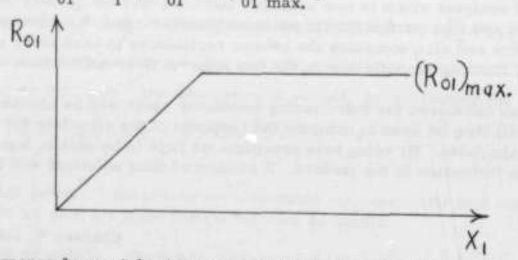


FIG. 3

The building response for each load is carried out to determine the maximum deflection of the lower mass and the maximum relative deflection between the two masses. New values of the load are calculated and tried until the load that causes the required deflections is found. We have devised a trial and error procedure for selecting the critical load from 64 possibilities with a maximum of six trials. The procedure starts with the middle value of the loading (#32) and then selects either the 16th value or the 48th value depending upon whether the calculated deflection is too high or too low. The procedure continuous to select middle values of the increasingly smaller groups until the critical loading is selected.

The program has been run for six different resistance values and has been checked by hand calculations. The data for the main part of the program is now being compiled and the problem should be completed by the end of March.

Charles W. Johnson

REACTOR RUNAWAY PREVENTION

In the past three months considerable progress has been made with calculations pertinent to the safety of the proposed M.I.T. Nuclear Reactor.

To meet a deadline some undesirable approximations had to be made, but since the calculations have been reorganized. It is expected that the more precise answers will be obtained soon.

During the next three months a new method will be developed which will make the calculations more useful and give more accurate answers.

Little progress was made on the relaxation calculation, mentioned in the last report, due to the urgency of the calculations mentioned above.

M. Troost

2.3 Final Reports

NEWTON ANALYSIS OF EARTH RESISTIVITY MEASUREMENTS

Very little has been published on direct interpretation of earth electrical measurements. This has probably been one of the major reasons for the periodic fluctuations of interest and activity which electrical work has undergone. In general, the problem of analysis of apparent resistivities to give actual resistivity distributions is a difficult one because the relations between the parameters of the distribution and the apparent resistivities are not only non-algebraic, they are non-linear as well. All existing interpretation methods, to to the extent of this writer's knowledge contain assumptions which simplify the physical situation and, therefore, the algebra. The analysis presented here is no exception. Some methods also contain assumptions of linearity. These latter assumptions can be, at best, very poor approximations in very exceptional cases.

The only published paper relating to direct, practical interpretation is that of Pekeris (1940), in which a graphical technique is developed for analysis of the Slichter kernel (Stefanesco, 1930) under the assumptions of any finite number of horizontal layers, each homogeneous, isotropic, and thicker than the one above it (Rogers, 1952). This method appears to work quite well in practical cases in which the assumptions, especially the last, are satisfied. It should be noted that the number of layers is yielded by this analysis.

The method presented here assumes a given (finite) number of horizontal layers, each isotropic and homogeneous, with no restrictions (other than those imposed by the physics) on the values of thicknesses and resistivities. Mathematically, it is an iterative solution to sets of non-linear algebraic equations in several variables. The actual amount of arithmetic involved in any one iteration is very large, and, as many as fifty iterations may be required for a solution. This method would have been impracticable before the advent of the high-speed digital computer. Even now some would think of this no more than an exercise in algebra. However, only by utilizing to the fullest these rapidly increasing computing facilities will progress in geophysical analysis be made.

The advantage of direct interpretation, as opposed to indirect approaches such as visual curve matching or model study, is seldom fully appreciated. It stems from the excessive sensitivity of the solutions of the kind of boundary value problem considered here to small changes in the boundary conditions. Stated inversely, this is a very poor sensitivity of the boundary values (potentials, apparent resistivities) to changes within the medium. This can be considered as low resolving power, and is brought out from one aspect in a discussion by

Morse (1953, p. 689). Thus, a very small difference between curves of, say, apparent resistivity can mean very great differences in actual conductivity distributions. Hence, if a quantitative interpretation with any degree of accuracy is desired, as in the case of detailed surveys, it is necessary that all the accuracy of the field data be utilized. As will be seen from the data presented here, even the full three or four place accuracy of field data often allows a fairly wide range of possible solutions. The obvious disadvantage of direct interpretation is the large amount of numerical work involved as compared with matching apparent resistivity curves.

The physical situation, as mentioned above, consists of the half-space $z \geqslant 0$ (circular-cylindrical coordinates) made up of a given finite number of strata parallel to the surface $z = 0$. Each stratum has thickness d_i and is homogeneous and isotropic with resistivity ρ_i ($i = 1, 2, 3$ --- n, $d_n = \infty$) (Fig. 1). On the surface of the half space, at $z = 0$, $r = 0$, is a point source of D.C. current, the sink being the hemispherical shell of radius $R = (r^2 + z^2)^{1/2} = \infty$. The quantity analyzed is the potential as a function of distance along the surface from the point current source, $\varphi(r)$.

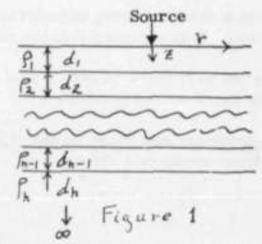


Figure 1

In any given field situation, the validity of the assumptions of parallel horizontal layering, homogeniety and isotropy, if not obvious, can be tested. There are certainly areas where these hold. The assumption of some given number of layers is not much of a limitation, since an excessive number can be assumed. The analysis should then give to the extra layers either resistivities equal to those of adjacent layers, or zero thicknesses. The determination of the effective φ (r) from apparent resistivity values is a simple matter, and is described by Mooney and Wetzel (1955).

Mathematical Analysis

In the case, as here, that resistivity is a function only of depth , the potential on the surface of the half-space can be expressed as (Stefanesco, 1930)

$$\text{(1)} \quad \varphi(r) = \int_0^\infty k(\lambda)\, J_0(\lambda r)\, d\lambda$$

where $k(\lambda)$ is a function determined by the way in which the resistivity varies with z, and λ, for the purposes of this description, can be called a parameter of integration. The function $k(\lambda)$, is called the Slichter kernel. For some special kinds of resistivity-depth functions, $k(\lambda)$ can be analytically determined in terms of the parameters of the function (Stefanesco, 1930; Slichter, 1933; Langer, 1933, 1936; Pekeris, 1940; Sunde, 1949; King, 1933). This is the case for stepwise variations, such as ours, and for real or imaginary exponential variations, among others. A systemic representation of $k_n(\lambda)$, the kernel for n layers, appears in Sunde (1949, p. 54).

$$\text{(2)} \quad k_n(\lambda) = [\,1 - \mu_{12\cdots n} t_1\,] \,/\, [\,1 + \mu_{12\cdots n} t_1$$

where

$$\mu_{12\cdots n} = \frac{\rho_1 - \rho_2 k_{23\cdots n}}{\rho_1 + \rho_2 k_{23\cdots n}}, \qquad k_{(m-1)m\cdots n} = \frac{1 - \mu_{(m-1)m\cdots n} t_{m-1}}{1 + \mu_{(m-1)m\cdots n} t_{m-1}}$$

$$\mu_{(m-1)m\cdots n} = \frac{\rho_{m-1} - \rho_m k_{m(m+1)\cdots n}}{\rho_{m-1} + \rho_m k_{m(m+1)\cdots n}}, \qquad t_m = e^{-2\lambda d_m}$$

This expression is obviously non-linear in all parameters.

Fortunately, equation (1) is a Hankel transform, and can be inverted to give

$$\text{(3)} \quad k(\lambda) = \lambda \int_0^\infty r\, \varphi(r)\, J_0(\lambda r)\, dr$$

This relation permits the evaluation of a Slichter kernel from a set of field measurements.

Numerical Analysis

The procedure followed, then, is to assume that n layers exist and that, therefore, the field kernel can be fitted by a kernel $k_n(\lambda)$, with the values of the parameters d_i and ρ_i yet to be determined. The field kernel $k(\lambda_j)$ is then evaluated for m values of λ_j*

$$m \geqslant 2n-1$$
$$j = 1, 2, ---, m$$

We then have m non-linear algebraic equations in (2n-1) unknowns, and the remaining problem is purely numerical. General methods for handling this problem are described in the literature (see, for example, von Sanden, 1923, or Householder, 1953). The method first used, and described here, is a combined Newton-Least Square solution.

Let the field kernel $k(\lambda)$ calculated for $\lambda = \lambda_i$ be $k(\lambda_i) = K_i$. Assuming an n-layered structure, and with initial estimates, $X_\ell^{(0)}$, of the parameters sought, X_ℓ,

$$k_n(\lambda_i, X_\ell^{(0)}) - K_i = k_{n_i}^{(0)} - K_i = \epsilon_i^{(0)}$$

and

$$k_n(\lambda_i, X_\ell) - K_i = k_{n_i} - K_i = 0$$

Here the X_ℓ are the ρ_i and d_i, with $\ell = 1, 2, ---, 2n-1$.** Likewise, for a second approximation to the parameters, $X_\ell^{(1)}$,

$$k_{n_i}^{(1)} - K_i = \epsilon_i^{(1)}$$

$$\epsilon_i^{(1)} - \epsilon_i^{(0)} = \Delta\epsilon_i^{(1)} = k_{n_i}^{(1)} - k_{n_i}^{(0)} = \Delta k_{n_i}^{(1)}$$

The further assumption is made that the kernel can be expanded in a Taylor Series about the value from any estimate, for example the first, i.e.

$$k_n(\lambda_i, X_\ell^{(0)} + dX_\ell) = k_{n_i}^{(0)} + \sum_{\ell=1}^{2n-1} \Big[\frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} dX_\ell + \frac{\partial^2 k_{n_i}}{\partial X_\ell^2}\Big)(dX_\ell)^2 \quad + \text{cross terms and higher derivatives} \Big]$$

In particular

$$K_i = k_{n_i}^{(0)} + \sum_{\ell=1}^{2n-1} \Big[\frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} (X_\ell - X_\ell^{(0)}) + \frac{\partial^2 k_{n_i}}{\partial X_\ell^2}\Big)_{X_\ell^{(0)}} (X_\ell - X_\ell^{(0)})^2 \quad + \text{cross terms and higher derivatives} \Big]$$

The Newton Method of first approximation then states

$$k_{n_i}^{(1)} = k_{n_i}^{(0)} + \sum_{\ell=1}^{2n-1} \frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} \Delta X_\ell^{(1)}$$

It is seen that this is an approximation which becomes more nearly exact as the second and higher derivatives, and cross derivatives, diminish in magnitude relative to the first derivatives, and that the statement is exact only in the case that the function is linear in its variables. Such is definitely not the case with the Slichter kernel, as is seen from equation 2. However, within a very small range even exponentials can be approximated by straight lines, and thus the implicit assumption is that the first estimates $X_\ell^{(0)}$ of the parameters are reasonably close to the true values X_ℓ.

----

*See the Appendix , or Mooney and Wetzel (1955). The latter is especially well suited to hand calculations.
**Actually, the values of ρ_1 and ρ_n are known from the asymptotic values of the apparent resistivity curve, and there are only (2n-3) unknowns.

Then

$$\Delta k_{n_i}^{(1)} = k_{n_i}^{(1)} - k_{n_i}^{(0)} = \sum_{\ell=1}^{2n-1} \frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} \Delta X_\ell^{(1)} = \Delta \epsilon_i^{(1)}$$

The standard Newton Method is to evaluate ϵ_i for (2 n-1) values of λ_i, and to calculate the $\Delta X_\ell^{(1)}$ by setting

$$\Delta \epsilon_i^{(1)} = \epsilon_i^{(0)}, \text{ etc}, \quad i = 1, 2, 3, \cdots 2n-1$$

or

$$\sum_{\ell=1}^{2n-1} \frac{\partial k_{n_1}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} \Delta X_\ell^{(1)} = \Delta \epsilon_1^{(1)} = + \epsilon_1^{(0)}$$

$$\sum_{\ell=1}^{2n-1} \frac{\partial k_{n_2}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} \Delta X_\ell^{(1)} = \Delta \epsilon_2^{(1)} = + \epsilon_2^{(0)}$$

$$\vdots \qquad\qquad \vdots$$

$$\sum_{\ell=1}^{2n-1} \frac{\partial k_{n_{(2n-1)}}}{\partial X_\ell}\Big)_{X_\ell^{(0)}} \Delta X_\ell^{(1)} = \Delta \epsilon_{2n-1}^{(1)} = + \epsilon_{2n-1}^{(0)}$$

and one has (2 n-1) linear equations in (2n-1) unknowns, the $\Delta_\ell^{(1)}$, which can be solved exactly, giving

$$X_\ell^{(1)} = X_\ell^{(0)} + \Delta X_\ell^{(1)} .$$

If no errors were present in the field data, and none were introduced in the (numerical) integration of K_i, then it could be expected that $k_n(\lambda_i, X_\ell)$ would exactly equal K_i. However, even barring departures of the geology from that assumed, errors do exist in all field data. Readings of voltage and current cannot be exact because of the limited accuracy to which meters can be read. Add to this the usual vagaries of field equipment, and it can probably be said that the K_i integrated from the best field data contain random errors in the third significant figure, and occasionally even in the second significant figure. As was discussed in the introduction, and as documented by the results, at times even the fifth or sixth place can determine changes in a solution that may be important when planning a drilling program. Thus, it is desirable to be able to eliminate the contribution of random errors, and this is the purpose of the Least Square modification. This formulation minimizes the function

$$\sum_{i=1}^{m} (\Delta \epsilon_i^{(s+1)} - \epsilon_i^{(s)})^2 , \qquad m > 2n-1$$

with respect to the ΔX_ℓ, viz:

$$\frac{\partial}{\partial \Delta X_\ell} \sum_{i=1}^{m} (\Delta \epsilon_i^{(s+1)} - \epsilon_i^{(s)})^2 = 0 \qquad \text{for all } \ell = 1, 2, \cdots 2n-1$$

$$\sum_{i=1}^{m} (\Delta \epsilon^{(s+1)} - \epsilon_i^{(s)}) \frac{\partial}{\partial \Delta X_\ell}\Big)_{X_\ell^{(s)}} (\Delta^{(s+1)} \epsilon_i) = 0$$

but, from above

$$\Delta \epsilon_i^{(s+1)} = \sum_{\ell=1}^{2n-1} \frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{s}} \Delta X_\ell^{(s+1)}$$

so that

$$\sum_{j=1}^{2n-1} \Delta X_j^{(s+1)} \sum_{i=1}^{m} \frac{\partial k_{n_i}}{\partial X_j}\Big)_{X_j^{(s)}} \frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(s)}} = \sum_{i=1}^{m} \epsilon_i^{(s)} \frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(s)}}$$

for each value of ℓ. This is, again, a set of (2 n-1) linear equations in (2 n-1) unknowns, the ΔX_ℓ. Summarized in matrix notation, these equations are

$$(4) \qquad [a_{\ell j}^{(s)}]\{\Delta X_j^{(s+1)}\} = \{b_j^{(s+1)}\}, \quad a_{\ell j}^{(s)} = \sum_{i=1}^{m} \frac{\partial k_{n_i}}{\partial X_j}\Big)_{X_j^{(s)}} \frac{\partial k_{n_i}}{\partial X_\ell}\Big)_{X_\ell^{(s)}},$$

$$\text{evaluated at } X_j^{(s)}, X_\ell^{(s)}. \qquad , \; b_j^{(s)} = \sum_{i=1}^{m} \epsilon_i^{(s)} \frac{\partial k_{n_i}}{\partial X_j}\Big)_{X_j^{(s)}} .$$

The question arises as to the behavior of the solution at minimum error, when this minimum value is greater than zero, and when, in particular, the largest portion of the error is due to a single point. Reference to equation 4 shows what will occur in this situation. The partial derivatives change very little over a small range of variation of the parameters, whereas the errors, ϵ_i, change relatively large amounts. When the kernel is too far from the erratic point, the large ϵ_i from that one point will dictate both the magnitudes and directions of parameter changes. As the error due to the erratic point is decreased, the errors due to the other points (which dictate parameter changes in the opposite direction) are increased until the net predicted changes are nil.

Computation Procedure

The foregoing was a rather complete statement of the problem and the attempted solution. A program was written for the Whirlwind I computer to handle the three-layer case. As mentioned in a footnote, in the practical case both ρ_1 and ρ_3 are known, hence the unknowns remaining are ρ_2, d_1, and d_2. The input data were:

a) the number and values of λ_i

b) the values ρ_1 and ρ_3, and the estimates of ρ_2, d_1 and d_2

and c) the K_i

For most cases, ten values of λ_i were used, in the range from $\lambda = 1.0$ to $\lambda = 0.006$. All resistivities were reduced to $\rho_1 = 1.0$, and ρ_2, d_1 and d_2 were estimated from the kernel behavior or from apparent resistivities.

Theoretical three and four-layer kernels and field kernels were analyzed. Several hundred theoretical kernels were calculated, with seven to eight place accuracy, on Whirlwind. Field kernels were integrated on Whirlwind, as described in the Appendix.

The machine calculated all the elements of the matrix, solved the matrix using Crout's method (Hildebrand, 1952, p. 503), determined the new values of the parameters, and returned to the beginning. It continued iterating until the error $\Sigma \epsilon_i^2$ began to make random oscillations, indicating no more possible improvement, or until the solution blew up, indicating one of several situations, to be discussed in the following sections.

Several practical computational difficulties should be mentioned. First, the kernel for the three layer case is (using the notation of Sunde, 1949, p. 55)

$$k_3(\lambda) = (1 - \mu_{123} t_1)/(1 + \mu_{123} t_1)$$

$$\mu_{123} = (\rho_1 - \rho_2 k_{23})/(\rho_1 + \rho_2 k_{23})$$

$$k_{23} = (1 - \mu_{23} t_2)/(1 - \mu_{23} t_2)$$

$$\mu_{23} = (\rho_2 - \rho_3)/(\rho_2 + \rho_3)$$

and

$$t_1 = e^{-2\lambda d_1}$$

$$t_2 = e^{-2\lambda d_2}$$

The algebra was simplified by using throughout

$$f_3(\lambda) = 1/(1 + k_3(\lambda)) - 1/2 = \mu_{123} t_1 / 2$$

instead of $k_3(\lambda)$.

Second, as will be seen from the results, the parameter changes calculated, especially at the beginning of the calculations, are almost always far too large. This necessitates an empirically determined parameter change multiplier, M, to prevent the solution from oscillating wildly. The reason for the overshoot, of course, lies in the departure of the kernel from the linear behavior postulated for it (see Hildebrand, 1949, p. 364). Second derivatives calculated were, indeed, quite large. The values settled upon for M were $\frac{1}{20}$ at the beginning of a calculation, increasing to 1.0 near the end. If a solution began to diverge after an increase of M, the next smaller value of M was brought back.

The Crout solution was used because it is economical of machine storage. It does not take advantage of the symmetry of the matrix, and thus would not be used in the case of more variables. Also, the accuracy is especially sensitive to the range of variation of the diagonal elements, and it was found quite important in some cases that each row be normalized by this element.

Another suggestion, although it was not followed in these calculations, is that once the solutions stop changing rapidly the derivatives need not be calculated at each iteration, but rather, the same values may be used for several iterations.

It is important to note that the kernels for very large and very small values of λ need not be considered, since these values will be monopolized by ρ_1 and ρ_3, respectively, which are treated as knowns.

Results

Analysis was attempted of 22 three layer cases, 3 four layer cases and 5 field cases.

The three layer kernels were all known to seven place accuracy. However, the analyses were done on data rounded off to three place accuracy, as would be the case for field data. In addition, several of the same cases were tested with more places of accuracy to observe the improvement in the solution. Rounding off the data in this fashion is equivalent to introducing a random error of range $\pm \frac{1}{2}$ in the last figure. Many of the cases chosen for analysis were moderately to very difficult in that either d_2 was much less than d_1, or the resistivity contrasts were low, or both. One quite interesting result, which is intuitively appealing, is that in the case of ρ_2 much greater or much less than ρ_3 there is a functional relationship between ρ_2 and d_2. When $\rho_2 >> \rho_3$, the product $\rho_2 d_2$, but not ρ_2 or d_2, can be found accurately. When $\rho_2 << \rho_3$, only the ratio ρ_2/d_2 can be determined to any degree of accuracy. That this should be the case can be seen from the asymptotic behavior of the expression for k_n.

In several of the cases presented, this procedure was unable to give a solution which was any better than the first estimate. This is probably due to irregularities on the error "surface", along which the iteration is proceeding, and could, in some cases, be eliminated by some other kind of procedure. To check this hypothesis, a modified "steepest descent" method was tried. Preliminary results indicate that this will help (see p. 40). More work is being done in this direction.

It will be noted in the results which follow that some kernels have been analyzed more than once. This has been done to investigate the reaction of the analysis to

a) changing the first estimates

b) changing the accuracy of the kernel

and c) changing the size of M, the parameter change multiplier

With regard to a), it was found that there exists a certain range, about true value, for each of the variables, within which the solution will be substantially the same regardless of the first estimates. Qualitative investigation of the size of this range leads us first to the question of uniqueness of the solution. It is the author's belief, although it has not been proven, that for completely accurate data only one physically allowable solution exists (excluding degeneracy, of course). That this is so for the three-layered case seems intuitively apparent, but it is not so obvious for the many-layered cases. Convergence of this analysis from any starting point whatever, as stated above, would require a smooth error "surface" (the multi-dimensional surface generated by the curves traced out by the error when varying one parameter at a time). The smoother (i.e., closer to first order) the surface, the larger the allowable M and the more rapid the convergence. Inflections or secondary minima in the surface, make machine solution of the problem much more difficult.

Increasing the accuracy of the kernel data in every case improved the quality of the solution, as expected. The amount of improvement can be seen in cases 9, 13, 14, 17 and 19.

At any step in the solution there is some optimum value of M which will give the largest decrease in error. To find this value, would require calculating the errors obtained using several different values of M and interpolating. Since the error calculation is the most time-consuming portion of each iteration, it is seen that such a procedure would be impractical. Instead, it was found empirically that a small M was required at the beginning of the solution, but that after about 15 iterations the process had stabilized sufficiently to allow much larger values of M to be used. The normal usage was M = .05 for the first 15 steps, .5 for the next 15, and then M = 1. In the event that a step gave a large increase of error, provision was made to bring back the result of the previous step and the next smaller value of M.

As a test of the stability of the procedure, three four-layer kernels were analyzed with the three-layer analysis. It is seen that the solutions are reasonable approximations to the true situations and that the final errors do not get as small as with the three-layer kernels. Also, converge is slower than is the case with three-layer kernels. The same general tendencies might be expected of field kernel analyses. A rather unexpected result is that this analysis (in these three cases) tends to ignore the third of the four layers.

The ultimate test of the method, of course, is what it will do with field data. Five such cases were tested. Figures 2, 3, and 4 show the apparent resistivities, integrated potentials, and kernels.

Case A did not satisfy the assumptions in two respects. First, the $r\phi(r)$ did not reach a constant value, and had to be smoothed artificially, and second, lateral variation existed as shown by the apparent resistivity curve (see Fig. 2) and by another taken in a direction perpendicular to that of the one shown. Drilling showed a good conductor at 6.2 units of depth and below. Note that the solution is degenerate.

Case B appeared to be a nearly ideal three-layer case. Drilling showed a good conductor at 5.0 units depth and below.

Case C from the apparent resistivity curves, would seem to be at least a four-layer case. No drill holes existed in the area.

Case D from the apparent resistivity, is very nearly a three layer case. The fit obtained is exceptional, but no drill holes exist.

Case E appears to be at least a four-layer case, however, the solution obtained degenerates to a two-layered case. No drill holes exist.

THREE-LAYER ANALYSIS OF FIELD KERNELS

Case	First Estimate				Solution			
	ρ_1 / d_1	ρ_2 / d_2	ρ_3	$\sum_{i=1}^{10} \epsilon_i^2$	ρ_1 / d_1	ρ_2 / d_2	ρ_3	$\sum_{i=1}^{10} \epsilon_i^2$
A	1. / .15	2.0 / 7.0	1.48	8.5×10^{-2}	1. / .145	1.53 / 271.3	1.48	2.4×10^{-4}
B	1. / .2	.6 / 4.	.2	1.7×10^{-3}	1. / .152	.641 / 2.68	.2	1.2×10^{-5}
C	1. / .5	.4 / 4.	.21	3.7×10^{-2}	1. / .271	.252 / 5.72	.21	1.7×10^{-4}
D	1. / .1	.75 / 2.	.175	1.2×10^{-2}	1. / .243	.708 / .882	.175	3.1×10^{-7}
E	1. / .2	.2 / 5.	.147	1.2×10^{-2}	1. / -1.70	1.00 / +2.23	.147	2.1×10^{-5}

THREE-LAYER ANALYSES OF THREE-LAYER KERNELS

Case	True Values				Solution					First Estimate				A**
	ρ_1 / d_1	ρ_2 / d_2	ρ_3	$\rho_2 d_2$ / d_2/ρ_2	ρ_1 / d_1	ρ_2 / d_2	ρ_3	$\sum_{i=1}^{10} \epsilon_i^2$	$\rho_2 d_2$ / d_2/ρ_2	ρ_1 / d_1	ρ_2 / d_2	ρ_3 / d_3	$\sum_{i=1}^{10} \epsilon_i^2$	
1*	1	1	1		1	1.00	1			1	2	1		8
	1	1			1.06	2.05		10^{-14}		1.2	.8		$2.4x10^{-2}$	
2	1	.1	10		1	.100	10			1	.5	10		4
	1	10		100	1.00	9.98		$7x10^{-8}$	100.	.75	25		$2x10^{-2}$	
3	1	.1	1		1	.105	1			1	.2	1		5
	1	1		10	.997	1.05		$5x10^{-7}$	10.0	1.2	.8		$3x10^{-2}$	
4	1	.1	10		1	.0994	10			1	.5	10		5
	1	1		10	1.00	.994		$4x10^{-7}$	10.0	.8	2		10^{-1}	
5	1	.05	5		1	$2.5x10^{-4}$	5			1	.01	5		3
	1	.5		10	1.12	? $2x10^{-3}$		$6x10^{-3}$	12.6	1.2	.3		.15	
6	1	10	.2		no solution					1	7	.2		3
	1	.5								.8	.3		$5x10^{-2}$	
7	1	.05	.2		1	.0480	.2			1	.1	.2		3
	1	.5		10	1.002	.485		$2x10^{-7}$	10.1	.9	.4		$2x10^{-4}$	
8	1	10	5	5	1	11.3	5		6.0	1	15	5		3
	1	.5			1.004	.424		$9x10^{-8}$		1.1	.4		$2x10^{-4}$	
9a	1	.05	5		1	.203	5			1	.02	5		3
	1	.1		2	.973	.412		$8x10^{-8}$	2.03	1.1	.2		.2	
9b	1	.05	5		1	.0888	5			1	.02	5		5
	1	.1		2	.996	.178		$5x10^{-11}$	2.00	1.1	.2		.17	
10	1	10	.1	1	1	20.9	.1		.978	1	20	.1		3
	1	.1			.645	.0468		$3x10^{-3}$		.6	.05		$3x10^{-3}$	
10***	1	10	.1	1	1	19.3	.1		1.01	1	20	.1		3
	1	.1			.987	.0524		$7x10^{-7}$		.6	.05		$3x10^{-3}$	
11	1	10	.2		no solution					1	5	.2		3
	1	.1								.9	.12		$5x10^{-3}$	
12	1	.5	10	.2	1	.992	10		.508	1	.2	10		3
	1	.1			.688	.504		10^{-6}		.75	.2		.014	
13a	1	.1	1		1	.436	1			1	.5	1		3
	1	.1		1	.903	.535		$8x10^{-8}$	1.23	1	.5		10^{-3}	
13b	1	.1	1		1	.0994	1			1	.5	1		8
	1	.1		1	1.000	.0994		$6x10^{-14}$	1.00	1	.5			
14a	1	10	1	1	1	5.98	1		1.02	1	5	1		3
	1	.1			.992	.171		10^{-10}		1.1	.6		$4x10^{-3}$	
14b	1	10	1	1	1	6.92	1		1.01	1	5	1		5
	1	.1			.996	.146		$7x10^{-8}$		1.1	.6		$4x10^{-3}$	
15a	1	2	.2		no improvement					1	.8	.2		3
	1	.1								.8	.2		10^{-6}	
15b	1	2	.2	.2	1	1.04	.2		.290	1	1.2	.2		3
	1	.1			.745	.279		10^{-4}		.8	.2		$5x10^{-4}$	

*Degenerate solution.

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

***Steepest Descent Analysis.

THREE-LAYER ANALYSIS OF THREE-LAYER KERNELS (Contd)

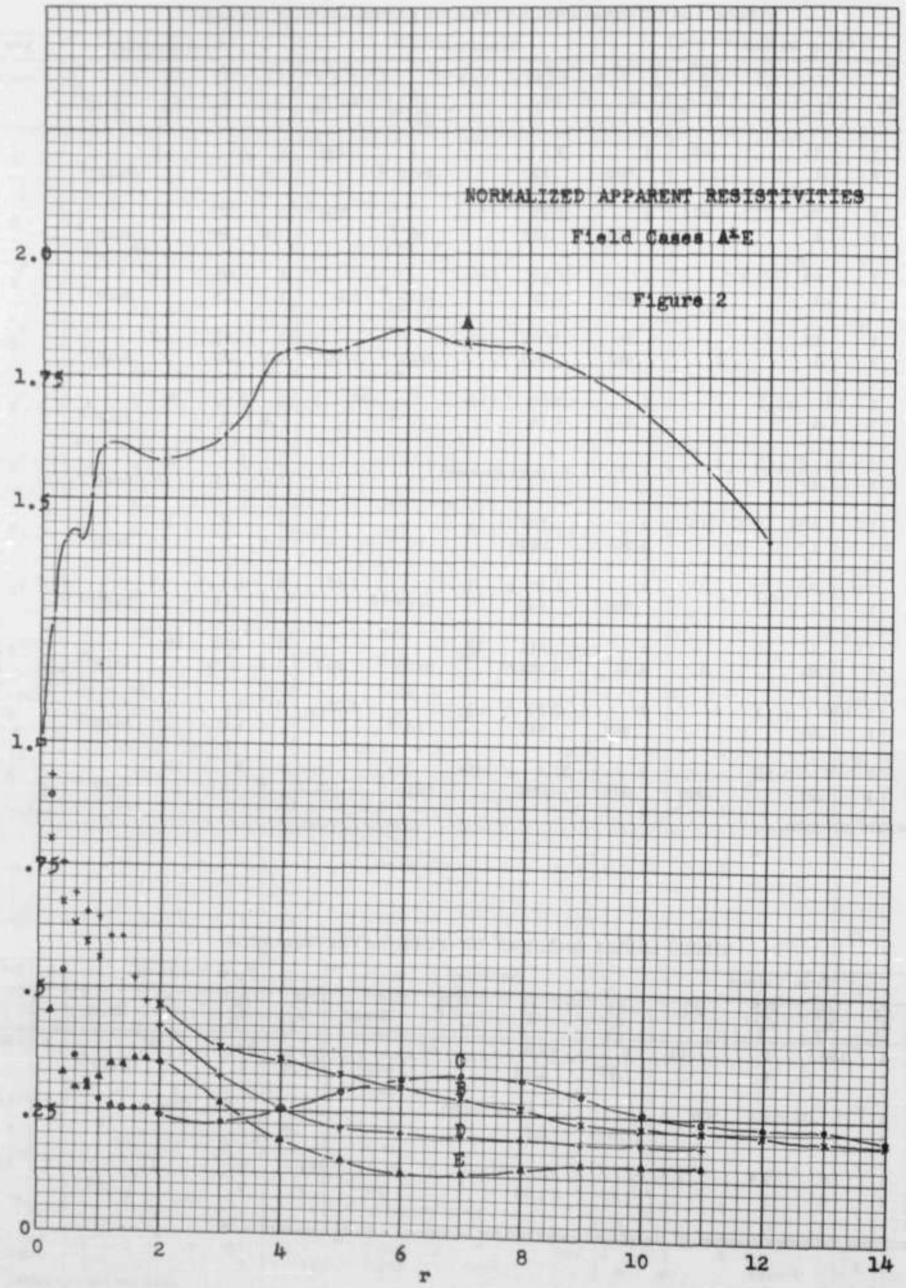
Case	True Values				Solution					First Estimate				A**
	ρ_1 / d_1	ρ_2 / d_2	ρ_3	$\rho_2 d_2$ / d_2/ρ_2	ρ_1 / d_1	ρ_2 / d_2	ρ_3	$\sum_{i=1}^{10} \epsilon_i^2$	$\rho_2 d_2$ / d_2/ρ_2	ρ_1 / d_1	ρ_2 / d_2	ρ_3 / d_3	$\sum_{i=1}^{10} \epsilon_i^2$	
16a	1	.75	.1	.075	1	3.3	.1		.429	1	5	.1		3
	1	.1			.802	.130		$2x10^{-3}$		.8	.1		$3x10^{-3}$	
16b	1	.75	.1	.075	1	1.87	.1		.290	1	.5	.1		3
	1	.1			.651	.155		10^{-3}		.8	.08		$5x10^{-3}$	
17a	1	.05	.2		1	.171	.2			1	.02	.2		3
	1	.1		2	.976	1.12		$3x10^{-6}$	6.6	1.1	.25		$8x10^{-4}$	
17b	1	.05	.1		.1	.075	.2			1	.02	.2		5
	1	.1		2	.997	.158		$4x10^{-6}$	2.11	1.1	.25		$8x10^{-4}$	
18a*	1	10	5	1	1	5.00	5		-36.	1	8	5		3
	1	.1			.917	-7.18		10^{-4}		.8	.5		$4x10^{-3}$	
18b	1	10	5	1	no improvement					1	9	5		3
	1	.1								1.1	.11		$5x10^{-4}$	
19a	1	1.5	1	.15	1	.708	1			1	.9	1		3
	1	.1			1.39	.0840		10^{-4}		1.2	.5		$2x10^{-3}$	
19b	1	1.5	1	.15	1	1.46	1		1.57	1	1.2	.1		5
	1	.1			.996	.108		$5x10^{-12}$		1.1	.08		$2x10^{-5}$	
20	1	.1	10		1	.012	10			1	.05	10		3
	1	.01		.1	3.51	$4.08x10^{-4}$		$8x10^{-3}$	.033	1.2	.05		$4x10^{-2}$	
21	1	100	1	1	1	2.20	1		1.20	1	5	1		3
	1	.01			.904	.543		10^{-5}		.8	1.6		$5x10^{-2}$	
22	1	2	10		1	31.4	10			1	3	10		3
	1	.01		.005	.976	-.003		$6x10^{-5}$	-.00011	.9	.1		$4x10^{-4}$	

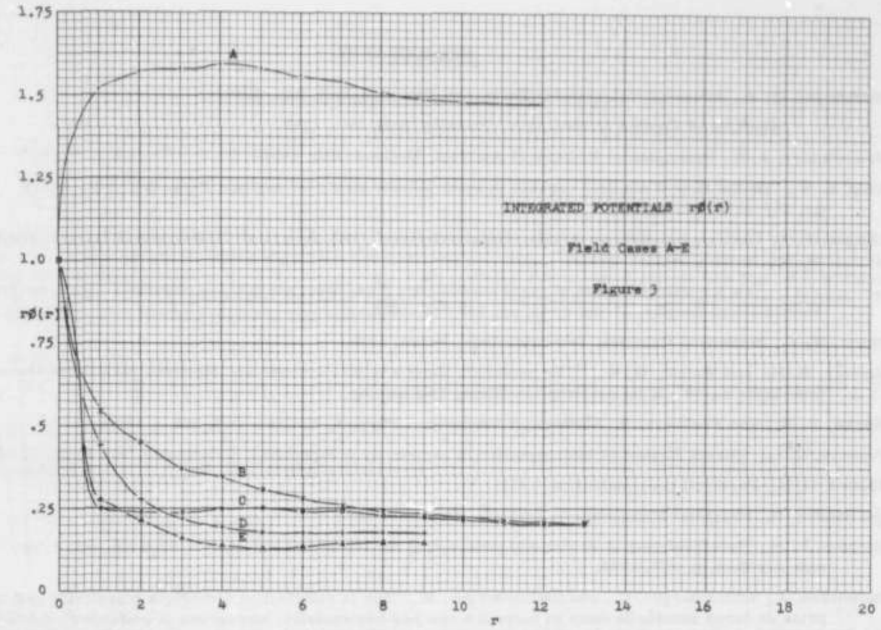
*Degenerate solution.

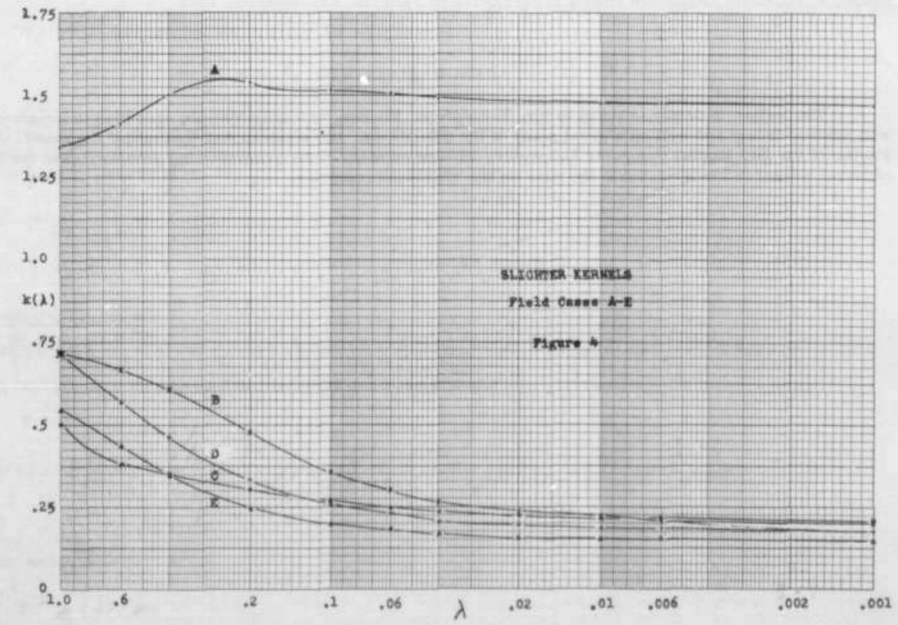
THREE-LAYER ANALYSIS OF FOUR-LAYER KERNELS

Case	True Values				Solution				First Estimate				A	B*
	ρ_1 / d_1	ρ_2 / d_2	ρ_3 / d_3	ρ_4	ρ_1 / d_1	ρ_2 / d_2	ρ_3	Error	ρ_1 / d_1	ρ_2 / d_2	ρ_3	Error		
23	1	100	1	.01	1	49.2	.01		1	50	.01		3	90
	1	1	4		.977	2.12		$4x10^{-5}$	.8	2		$2x10^{-3}$		
24	1	.01	1	100	1	.0252	100		1	.05	100		3	50
	1	1	4		.987	2.65			.8	1		.4		
25	1	10	1	.1	1	10.7	.1		1	5	.1		3	84
	1	4	1		1.05	3.63		10^{-3}	2	5		.07		

*This column indicates number of iterations required for solution, with M constant =.05.


NORMALIZED APPARENT RESISTIVITIES
Field Cases A-E
Figure 2
A
B
C
D
E
2.0
1.75
1.5
1.0
.75
.5
.25
0
0
2
4
6
8
10
12
14
r


INTEGRATED POTENTIALS $r\phi(r)$
Field Cases A-E
Figure 3
A
B
C
D
E
1.75
1.5
1.25
1.0
$r\phi(r)$
.75
.5
.25
0
0
2
4
6
8
10
12
14
16
18
20
r


SLICHTER KERNELS
Field Cases A-E
Figure 4
A
B
C
D
E
1.75
1.5
1.25
1.0
$k(\lambda)$
.75
.5
.25
0
1.0
.6
.2
.1
.06
λ
.02
.01
.006
.002
.001

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ACKNOWLEDGMENTS

The writer is deeply grateful to Mr. Theodore R. Modden, who suggested the approach to the problem and who advised freely and well on a great many of the difficulties. His ideas appear throughout the paper. Mr. Jack Porter of the MIT Digital Computer Laboratory advised on many of the programming problems, and the Office of Naval Research made available the time on the Whirlwind computer.

APPENDIX

Numerical Integration of the Slichter Kernel

The procedure used to integrate

$$k(\lambda) = \lambda \int_0^\infty r\varphi(r) J_0(\lambda r)\, dr$$

was as follows. The potential data $r\varphi(r)$ were given for a finite number of points, r_j. These are usually at 30, 50, or 100 foot intervals, depending on the electrode spread used. The assumption of three layers dictates that beyond a certain distance, r_c ($r_c >> d_1 + d_2$) the potential fall off shall behave like that on a uniform medium of resistivity ρ_3, and should therefore vanish as $\frac{1}{r}$. Thus beyond r_c, $r\varphi(r)$ should be constant. The value of this constant is determined in this fashion:

$$\frac{\varphi(r_j)}{r_{j+1}} = \frac{\varphi(r_{j+1})}{r_j}$$

$$\varphi(r_j) - \varphi(r_{j+1}) = \Delta\varphi_j$$

The quantities r_j, r_{j+1}, and $\Delta\varphi_j$ are measured, and

$$\varphi(r_j) = \frac{r_{j+1}}{r_j}[\varphi(r_j) - \Delta\varphi_j]$$

$$= -\frac{r_{j+1}}{r_j}\Delta\varphi_j \Big/ \left[1 - \frac{r_{j+1}}{r_j}\right]$$

φ was extrapolated to $\varphi_{(o)}$ by eye. Data from 20 equally-spaced values of r were used, including r = 0 and r = r_c. The data were replaced by two sets of fifth order orthogonal polynomials (see Milne, 1949, p. 265, ff.), one fitted to the last 15 points, the other to the first 6 points, where changes were more rapid. These then gave two series which represented the $r\varphi(r)$ in the intervals named

$$r_j\varphi(r_j) \simeq c_0 + c_1 P_5^1 + c_2 P_5^2 + \cdots + c_5 P_5^5 \equiv P_1 \quad , \quad j = 0, 1, 2, 3, 4, 5$$

$$r_j\varphi(r_j) \simeq d_0 + d_1 P_5^1 + d_2 P_5^2 + \cdots + d_5 P_5^5 \equiv P_2 \quad , \quad j = 5, 6, \cdots 19$$

Rearranging by powers of r

$$P_1 = g_0 + g_1 r + g_2 r^2 + \cdots + g_5 r^5 \quad , \quad j = 0, 1, \cdots, 5$$

$$P_2 = h_0 + h_1 r + h_2 r^2 + \cdots + h_5 r^5 \quad , \quad h = 5, 6, \cdots, 19$$

The integral becomes

$$k(\lambda) \simeq \lambda \int_0^{r_5} P_1(r) J_0(\lambda r)\, dr + \lambda \int_{r_5}^{r_{19}} P_2(r) J_0(\lambda r)\, dr + \lambda r_{19}\varphi(r_{19}) \int_{r_{19}}^{\infty} J_0(\lambda r)\, dr$$

where, of course, it is assumed that r φ(r) is constant beyond

r = r_c.

$$k(\lambda) = \lambda \sum_{\ell=0}^{5} g_\ell \int_0^{r_5} r^\ell J_0(\lambda r)\, dr + \lambda \sum_{\ell=5}^{19} h_\ell \int_{r_5}^{r_{19}} r^\ell J_0(\lambda r)\, dr + \lambda r_{19}\varphi(r_{19}) R_{19}$$

$$R_{19} = \int_{r_{19}}^{\infty} J_0(\lambda r)\, dr$$

But the integral

$$\int_a^b r^\ell J_0(\lambda r)\, dr$$

can be evaluated anaItyically, viz:

$$\int_a^b J_0(\lambda r)\,dr = \frac{2}{\lambda}\Big[J_1(\lambda r) + J_3(\lambda r) + J_5(\lambda r) + \cdots \Big]_a^b$$

$$\int_a^b r J_0(\lambda r)\,dr = \frac{1}{\lambda^2} J_1(\lambda r) \Big]_a^b$$

$$\int_a^b r^2 J_0(\lambda r)\,dr = \frac{1}{\lambda^3}\Big[r^2\lambda^2 J_1(\lambda r) + r\lambda J_0(\lambda r) - 2\big(J_1(\lambda r) + J_3(\lambda r) + J_5(\lambda r) + \cdots\big)\Big]_a^b$$

$$\int_a^b r^3 J_0(\lambda r)\,dr = \frac{1}{\lambda^4}\Big[\lambda^3 r^3 J_1(\lambda r) - 2\lambda^2 r^2 J_2(\lambda r)\Big]_a^b$$

$$\int_a^b r^4 J_0(\lambda r)\,dr = \frac{1}{\lambda^5}\Big[(\lambda r)^4 J_1(\lambda r) - 3(\lambda r)^3 J_2(\lambda r) + 3(\lambda r)^2 J_3(\lambda r) + 3\lambda r J_4(\lambda r) + 18\big(J_5(\lambda r) + J_7(\lambda r) + J_9(\lambda r) + \cdots\big)\Big]_a^b$$

$$\int_a^b r^5 J_0(\lambda r)\,dr = \frac{1}{\lambda^6}\Big[(\lambda r)^5 J_1(\lambda r) - 4(\lambda r)^4 J_2(\lambda r) + 8(\lambda r)^3 J_3(\lambda r)\Big]_a^b$$

etc.

The J_n were calculated by the machine using, at most, thirty terms of the series. It was found important that they be quite accurate in absolute value, since some of the coefficients q_ℓ and h_ℓ are very large. If a standard set of values of λ were decided upon, it would have been advantageous to tabulate the values of the functions.

Then

$$k(\lambda) = \sum_{i=0}^{5} K_i(\lambda, r_5, r_{19}, q_j, h_j)\, J_i(\lambda r_5) + \sum_{i=0}^{5} \eta_i(\lambda, r_5, r_{19}, q_j, h_j)\, J_i(\lambda r_{19})$$
$$+ r\gamma_1\big[\varphi(r_{19}, q_0, q_2, q_4, h_0, h_2, h_4, \lambda, r_5, r_{19})\big]\sum_{i=3}^{\infty} J_{2i+1}(\lambda r_5) + 2\gamma\big[h_0, h_2, h_4, \lambda, r_{19}, \varphi(r_{19})\big]\sum_{i=3}^{\infty} J_{2i+1}(\lambda r_{19})$$

Since all work was restricted to $\lambda r_{19} \le 38\ (\lambda \le 2)$, the first thirty terms of the series were always adequate for the calculation of $J_n(\lambda r_{19})$.

3. ACADEMIC PROGRAM

3.1 Institute Courses and Seminars

MACHINE-AIDED ANALYSIS

Sixty-one students attended the electrical engineering course 6.25 entitled Machine-Aided Analysis which was offered first semester, 1954. The course, under the supervision of Dr. W. K. Linvill, Associate Professor of Electrical Engineering, was given jointly by Profs. Linvill, R.C. Booton, and C. W. Adams.

Both analog and digital computational techniques were studied, as well as the numerical analysis and the solution of engineering problems by numerical methods. Although the emphasis was on typical engineering problems, some business problems were taken up also.

As practice in analog computational techniques, the facilities of REAC (Reeves Electronic Analog Computer) of the Servomechanisms Laboratory at MIT were used by the students for the solution of an ordinary differential equation.

In connection with the study of digital computational techniques, a problem (see Problem #221 in Part II of the present report) was programmed by each student for TAC, the summer session Three Address Computer. The facilities of the Digital Computer Laboratory were used by the students for the preparation of their routines. Time was made available for each student to be present at the running of his routine, for the correction of mistakes, and for the re-running of the routine.

INTRODUCTION TO DIGITAL COMPUTER CODING AND LOGIC

Sixty-five students are enrolled in course 6.535, Introduction to Digital Computer Coding and Logic, being given second semester, 1955, by Mr. D. N. Arden, Staff member of the Scientific and Engineering Computation Group of the Digital Computer Laboratory. The course will survey arithmetical algorithms used by high-speed digital computers and a discussion will be given concerning representation of numbers using an arbitrary base and the conversion of numbers from one base to another. A brief description of the logical design of a simplified computer, practice in writing subroutines, and the design of an interpretive code will also be given. Illustrations of some important mathematical techniques in the practical application of high-speed computers will also be considered. The students will be given practice in the practical coding of some of these techniques by using a simplified computer simulated by the MIT Whirlwind I computer.

NUMERICAL ANALYSIS

This year, for the first time, Professor Hildebrand is giving a second semester course in Numerical Analysis, M412. This semester the content of the course is 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

The biweekly seminar for the project reported in Part I of the present report has continued into the second semester of the academic year. Its purpose and place in the educational program of the project was fully outlined in the past quarterly report under the section headed Group Activities.

3.2 Group Activities

NUMERICAL ANALYSIS DISCUSSION GROUP

A group made up of (1) numerical analysis representatives of the Committee on Machine Methods of Computation and (2) mathematicians of the Digital Computer Laboratory have continued to meet informally as was reported last time. Some of the discussions have been a continuation of last semester's topics (see previous report) and a few have centered around the ideas that compose the first progress report of the present publication. Further new ideas or results that the group might contribute to, discuss, or criticize will be published in later progress reports under the same title, "A Study of the Basic Problem of Numerical Analysis Expressed in the Language of Computing Machines".

ACADEMIC PROGRAM

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 discussed in the appropriate progress report, section 2.2, Part I.

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 the homework problems are being 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 December 26, 1954 to March 20, 1955. During this time 66 problems made use of 326.27 hours of the 461 hours of Whirlwind I computer time allocated to the Scientific and Engineering Computation (S&EC) Group. These problems cover some 15 different fields of applications. The results of 22 of the problems have been or will be included in academic theses. Of these, 19 represent doctorate theses, two master's, and one Electrical Engineering. Thirty-seven 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 percent 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 is interesting to note that no programmer has reported difficulties due to machine malfunction or mistakes in service routines. In particular, 97% of the assigned machine time was usable.

Even though no major modifications were introduced into the comprehensive system of service routines, the development of new coding techniques by the S&EC Group was extended by the development of translation programs for MIT's Numerically Controlled Milling Machine and for the use of members of the Servomechanisms Laboratory in coding for the Univac Scientific 1103 computer.

Field	Description	Problem Number	%WWI Time	Source
Aeronautical Engineering	Low aspect ratio flutter	177, C	.16	MIT
	Blast response of aircraft	183, D	6,98	MIT
	Helicopter rotor stability	222, C	.79	MIT
	Transient response of aircraft structures to aerodynamic heating	236, C	1,07	MIT
Chemical Engineering	Six-component distillation variable enthalpy and equilibrium data	*130, B,N	.38	MIT
	Transient effects in distillation	*167, D	.53	MIT
	Reactor runaway prevention	*231, C	1,88	MIT
	Transients in distillation columns	241, B,N	1,38	MIT
Civil Engineering	Response of a five story frame building under dynamic loading	*203, C	.39	MIT
	Dynamic analysis of bridges	230, C	1,74	MIT
	Analysis of two story steel frame building	*252, N	.33	MIT
Electrical Engineering	Dynamics and control of packed distillation columns	251, B	.55	MIT
Geology and Geophysics	Geophysical data analysis	106, C	2,34	MIT
	Interpretation of earth-surface resistivity measurements	*123, C	2,33	MIT
	Dispersion curves for seismic waves	*212, C	1,47	MIT
Instrumentation Laboratory	An interpretive program to accept mathematical symbols	108, C	.86	MIT
	Servo response to a cosine pulse	211, C	.44	MIT
	Autocorrelation function of submitted data	237, C	.13	MIT
	Guidance and control	239, C	2,95	MIT
	Data reduction for X-1 fire control	244, C	.51	MIT
	Flight path of an aircraft during pullup	263, C	.16	MIT
Hydrodynamics Lab	Investigation of turbulent flow	223, B,N	.24	MIT
Lincoln Laboratory	Tracking response characteristics of the human operator	186, B,L	.09	MIT
	Eigenvalue problem for propagation of E.M. waves	193, L	1,27	MIT
Mathematics Department	Number of structures of relations on finite set	*242, N	.18	MIT
Mechanical Engineering	Flow of compressible fluids (aerothermopressor)	120, D	1,70	MIT
	Laminar boundary layer of a steady, compressible flow in the entrance region of a tube	199, C	1,96	MIT
	Evaluation of difference diffusion equation	*228, A	.52	MIT
Meteorology	Synoptic Climatology	155, D	9,89	MIT
	Distribution of gustiness in the free atmosphere	189, C	.12	MIT
	Computations of the fields of vertical velocity and horizontal divergence	224, N	5,36	MIT
	Surface pressure prediction	247, C	1,05	MIT
Physics Department	Coulomb wave functions	*122, B,N	2,89	MIT
	Self-consistent molecular orbitals	144, N	2,30	MIT
	Determination of phase shifts from experimental cross-sections	162, N	.07	MIT
	Overlap integrals of molecular and crystal physics	*172, B,N	3,71	MIT
	An augmented plane-wave method as applied to sodium	194, B,N	3,00	MIT
	Study of the ammonia molecule	201, N	.38	MIT
	Exchange integrals between real Slater Orbitals	204, N	3,25	Univ. of Chicago
	Variation-perturbation of atomic wave function and energies	*217, N	.50	MIT
	Transformation of integrals for diatomic molecules	218, N	.27	MIT
	Neutron-deuteron scattering	*225, B,N	1,97	MIT
	Atomic integrals	234, N	.22	MIT
	Eigenvalues for a spheroidal square well	*235, B,N	1,72	MIT
	Self-consistent calculation of nuclear mass density	*238, B,N	3,50	MIT
	Theory of neutron reactions	245, N	.03	MIT
	Energy levels of diatomic hydrides	260, N	.18	MIT
	Evaluation of two-center molecular integrals	262, N	.15	MIT
	Application of augmented plane wave method to chromium crystal	285, B,N	.17	MIT
Servomechanisms Laboratory	Data reduction program; polynomial fitting	126, C	5.12	MIT
	Subroutine for the numerically controlled milling machine	132, C	.21	MIT
	Translation program for the numerically controlled milling machine	250, C	.22	MIT
School of Industrial Management	Utility stock prices	233, C	.19	MIT
Dynamic Analysis & Control Laboratory	Flight interceptor control	249, C	.46	MIT
	Dynamic analysis of an aircraft interceptor	258, C	.11	MIT
Lab. for Nuclear Science	Energy levels in a spheroidal potential	232, B	.21	MIT
Research Lab. for Electronics	Plant surveys for control systems by statistical methods	215, B	.06	MIT
	Crystal filters	343, D	.04	MIT
Miscellaneous	Comprehensive system of service routines	100	11,58	MIT
	Special problems (staff training, etc.)	131	2,30	MIT
	Library of subroutines	141	1,06	MIT
	Intestinal motility	195, C	.80	Mass. Mem. Hospitals
	Single address computer	196	.22	MIT
	Comparison of simplex and relaxation methods in linear programming	219	.66	MIT
	Course 6.25, Machine-aided analysis	221, B	.19	MIT
	WWI-ERA 1103 translation program	256, C	2,51	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.
Matrix equation	Crout's method	177 C.
Eigenvalues	Iteration and diagonalization	201 N.
Zeroes of a matrix equation	Interpolation	*212 C.
Minimize an analytic equation	Basic arithmetic operations	*217 N.
Orthonormalization	Schmidt process	218 N.
Eigenvalues	Diagonalization	232 B.
2. Ordinary differential equations		
General system	Gill's modified fourth-order Runge-Kutta	108 C.
Seven nonlinear first order	Fourth-order Runge-Kutta	120 D.
Set of nonlinear first order equations	Second-order Runge-Kutta	*167 D.
Two second order	Extrapolation of differences	183 D.
System	Gill's method	199 C.
Five nonlinear second order	Difference equation	*203 C.
Second order linear	Power series	211 C.
Second order nonlinear	Rectangular integration	221.
Two linear second order with periodic coefficients	Fourth order Runge-Kutta	222 C.
Second order linear	Difference equation	230 C.
Set of first order equations	Gill's method	239 C.
Set of nonlinear first order equations	Second order Runge-Kutta	241 B,N.
Wave equation	Milne predictor-corrector formula	245 N.
Set of thirteen first order equations	Gill's method	249 C.
Nonlinear second order	Finite differences	252 N.
Set of eight first order equations	Gill's method	258 C.
Five equations with 30 sets of initial conditions	Gill's method	263 C.
3. Partial differential equations		
Schroedinger's equation	Summation of series	*122 N.
Diffusion equation	Recurrence formula	*228 N.
Schroedinger's equation in sph. coord. with non-separable potential	Matching wave functions at the boundary	*235 B,N.
Second order parabolic	Explicit finite differences	236 C.
First order linear set	Finite differences	251 B.
4. Integration		
Integral evaluation	Trapezoidal rule	*123 B,N.
Overlap integrals	Evaluation of analytic forms	*172 B,N.
Calculation of transfer functions	Simpson's rule	186 B,L.
Autocorrelation and Fourier transform	Simpson's rule	189 C.
Autocorrelation and Fourier transform	Simpson's rule	195 B,N.
Integral evaluation	Gaussian quadratic	204 N.
Auto- and crosscorrelation	Simpson's rule	215 B.
Stationary point of a variational	Simpson's rule	*225 B,N.
Integral transformation	Algebraic recursion formula	234 N.
Autocorrelation	Simpson's rule	237 C.
Hartree-Fock equations	Trapezoidal plus variational	238 B,N.
Overlap integrals	Evaluation of analytic forms	260 N.
Overlap integrals	Evaluation of analytic forms	262 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.
Regression analysis	Modified Doolittle method	233 C.
Numerical prediction	Quadratic approximation	247 C.
6. Transcendental equations		
Curve fitting	Iteration using least squares	162 N.
System of 47 equations	Step-by-step	*231 B,N.
7. Data Reduction		
General data reduction	Polynomial fitting, etc.	126 C.
Miss distribution	Arithmetic operations	244 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. Linear Programming		
Linear programming	Cyclic projections and simplex method	219

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 66 problems described below, twenty-six (219, 223, 224, 233-239, 241-245, 247, 249-252, 256, 258, 260, 262, 263, and 285) represent new problems that are being described for the first time. Ten problems (123, 130, 167, 183, 186, 189, 211, 222, 254, and 249) have been completed.

Tables 2-I and 2-II have been set up to provide the reader with a convenient <u>index</u> 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 per cent of the S&EC Group's WWI problem time (326.27 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 <u>NOT</u> for academic credit, is <u>UN</u>sponsored.

B implies the problem <u>IS</u> for academic credit, is <u>UN</u>sponsored.

C implies the problem is <u>NOT</u> for academic credit, <u>IS</u> sponsored.

D implies the problem <u>IS</u> for academic credit, <u>IS</u> 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&EC Group.

No major changes have been introduced into the comprehensive system of service routines (Problem 100). However, certain conveniences such as the inclusion of program annotations on the Flexowriter tape, optional suppression of the floating address table, use of automatic scope output requests, and improvements in the logging procedures have been incorporated.

Members of the S&EC Group have been active in the development of special pseudo codes and translation routines for the MIT Numerically Controlled Milling Machine (Problem 250) and the Univac Scientific Model 1103 (Problem 256).

2.2 Problems Being Solved

100. COMPREHENSIVE SYSTEM OF SERVICE ROUTINES

The comprehensive system of service routines has been developed by the Scientific and Engineering Computation (S&EC) Group to simplify the process of coding for WWI. The system now in use, called CS II, was described in Summary Reports No. 36, 37, and 38.

CSII provides for: 1) the direct read-in of Flexowriter-coded perforated paper tapes; 2) the logging of each problem on film and paper tape for subsequent processing; 3) assembly during read-in of a suitable set of instructions including interpretive programmed-arithmetic (with an optional floating-point number system), up to several hundred cycle counters (B-boxes), output routines, error detection, and automatic post-mortems.

Routines are normally coded with mnemonic operations, symbolic addresses, relative addresses, program and preset parameters, special pseudo-codes, and special control words. The service routines are permanently stored on magnetic tape and are transferred to a magnetic drum for automatic selection during read-in.

No major revisions were made during this quarter in the logic of CS II. However, the following improvements have been incorporated.

<u>Comment Words</u>

The CS conversion program has been modified so that comments can be typed on a Flexowriter tape along with the words in the coded program. A comment must be preceded by a vertical bar and terminated by a carriage return. Comments are ignored by the conversion program. For example,

```
si 78     |Select magnetic tape unit 1.
ca al
rc        |Record a word.
```

<u>Revision of Automatic Output Routines</u>

The automatic output routines DIB, DOB, iDIB and iDOB have been rewritten and shortened in the process. The programs have been modified to include recording on and reading from the buffer drum.

<u>Flad Table Suppression</u>

Printing of a floating address (flad) table as a result of a CS conversion can now be suppressed at the option of the programmer. This can be done either by using the word <u>ef,</u> in a director tape or by setting up a number in the selector panel and using the manual read-in mode.

<u>Modification of the Logging Program</u>

The logging program has been modified so that time entries are made in the log both at the beginning of a magnetic tape search for a utility program and at the termination of the read-in of the utility program. The resulting time increment will be subtracted from the total run-time for a problem by the automatic biweekly program.

<u>Modification of the Stop Instruction</u>

The STOP instruction has been modified to make a time entry in the log whenever one is executed. The exact time at which a program was completed is thus known.

<u>Modification of the Title Recording Program</u>

Tape titles have been recorded for delayed printing by the utility control program whenever CS Flexo (fc) tapes or post-mortem request (fp) tapes are read in. The program has been modified so that the date and time will be recorded along with the title.

The reference date and time are recorded on the buffer drum by the operators at the beginning of the computer operating period. An automatic indexing of the date occurs if the operating period extends beyond 2400 hours.

<u>Automatic Biweekly Program</u>

An automatic biweekly program has been written which will process all logging tapes produced during a biweekly period and produce a typed summary of computer operation for that period.

The typed summary consists of:

1. time used by each problem
2. lost time due to machine malfunction
3. accumulation of all the time used by all the problems
4. time used for checking auxiliary equipment
5. number of problems run
6. number of programs run
7. unused time (time between runs).

This program will automatically deduct time due to operator's errors, tape room errors, etc. It will also deduct time used for searching purposes, for instance searching for CS II or the scope post-mortem on magnetic tape. This program will print on the direct Flexowriter the date and initial time each logging tape started.

The use of logging tapes has reduced the time needed to prepare the S&EC biweekly report from more than 15 hours to about 20 minutes. This new procedure has eliminated most of the day-by-day clerical work that was needed to prepare the records pertinent to the biweekly statistics.

The time used in preparing the biweekly program is logged under problem 100. The logging routines will continue to be studied with regard to increasing their flexibility and functions. In particular it is planned to include in these routines the actual billing for non-ONR, non-Lincoln sponsored projects.

<u>Automatic Scope Output Requests</u>

The automatic output instruction SOA (iSOA), <u>S</u>cope <u>O</u>utput <u>A</u>lphanumerical, was made available to programmers using CS II. The special instructions COLUMN iCOLUMN and FRAME iFRAME were also introduced. A detailed description of these instructions may be found in Memorandum DCL-48.

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 to seismic record interpretations, and in particular to the separation of "reflections" from background interference on these records. More complete descriptions of the problem and the approaches used are contained in the bi-weekly report of June 15, 1953 (M-2244) and in "Detection of Reflections on Seismic Records by Linear Operators". (Wadsworth, Robinson, Bryan, and Hurley -- GEOPHYSICS, Vol. 18, No 3 July 1953).

The most recent approach to our problem has been a study of the statistical nature of the interference mentioned above and its relation to the physical mechanisms of generation. The hope is that this study should provide a basis for developing and for evaluating existing procedures of noise removal.

Computationally we are dealing with the functions of generalized harmonic analysis - correlation, spectra, coherency, linear operations, on discrete multiple time series. Computational details are given in previous summary reports. Estimates of these quantities on actual data are compared with theoretical and experimental estimates on truly stationary series, and interpreted in the light of various types of decomposition.

We have demonstrated that seismic interference approximates stationary series, but that the "stationarity" may have a wide range of type, ranging from absolute continuity of the integrated power spectrum to nearly step function behavior of the spectrum. An observed example of this latter extreme was explainable in terms of classical theory, an explanation which was found to be entirely in accord with the statistical explanation in terms of decomposition. We have also been able to explain certain problems in noise removal, and develop new techniques from the understanding we have gained.

Research reports are sent to a restricted group of supporting companies, but reproductions may be obtained through the special collection division of the M.I.T. Hayden Library, six months after the reports are sent to the companies. Occasionally papers are published in GEOPHYSICS.

The programming has been done by S. Simpson, D. Grine, S. Treitel, and I. Calnan, all of whom are associated with the MIT Department of Geology and Geophysics.

108 C. AN INTERPRETIVE PROGRAM

This problem is aimed at the development of a set of algebraic routines for Whirlwind I; i.e., a set of routines permitting the translation by Whirlwind of a problem stated in algebraic notation. Principal programmers are at present J. H. Laning, Jr. and C. Block of the MIT Instrumentation Laboratory.

Due to the pressure of other more urgent work, small progress has been made on this problem during the past quarter. At present, programs have been written for the execution of two preliminary scans of an

algebraically coded tape, in order to screen out details and leave the way open for a reasonably straightforward logical scan. The logical scan is itself only partially complete, however. In addition, much work remains to be done on the detailed routines for many of the special features to be provided in the new system. It is currently expected that active work on this problem will resume about the middle of the next quarter.

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 non-linear, first-order differential equations.

During the past quarter, a completely revised Whirlwind program treating the aerothermopressor analysis was completed and checked by systematic testing. This program, the writing of which began December 1, 1954 and required approximately ten weeks, involves the use of 5370 registers. The speed of computation, compared with the original program, written in early 1953, has been increased from four to six-fold, the latter figure for the situations in which a special wet-bulb temperature computation is required. This has been accomplished by elimination of interpretive programming wherever possible.

This program is directed by a single parameter tape, which will eventually be prepared by filling out a standard form, and therefore represents an automatic computation facility for the aerothermopressor. Some of the features of the program are:

1) Inclusion of five different numerical methods for solving the differential equations. These are (a) Euler method, (b) backward differences, (c) second-order Runge-Kutta, (d) fourth-order Runge-Kutta, and (e) forward and successive differences. The computations may be directed to change from one method to another arbitrarily.

2) Provision for automatic change of increment (according to an arithmetic progression) at each step, if desired.

3) Automatic detection and elimination of oscillations in liquid velocity.

4) Determination of singular solutions of the equations by a completely automatic iterative procedure. (This procedure, which requires about 5 minutes per solution, originally required about 30 minutes with the need of intermediate hand computations). Early stages of the iteration use the Euler method with an automatic change to fourth-order Runge-Kutta when more accuracy is required.

It is planned to resume computations on a broad scale. Considerable experimental data from the medium-scale aerothermopressor test facility is now available for corroboration of the analysis. Further, several procedures for calculating optimum performance of the aerothermopressor and for studying the effect of variations in droplet spectrum await exploitation.

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.

122 N. COULOMB WAVE FUNCTIONS

A report on this problem is given in section 2.2 of Part I.

123 N. EARTH RESISTIVITY INTERPRETATION

A report on this problem is given in section 2.2 of Part I.

126 C. 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 Walter Whelan 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 requires 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 for computer to operator communication and manual intervention registers so that the operator can communicate with the computer. The intent is to allow the human operator to 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 current version of the prototype data-reduction program is called the Basic Evaluation Program.

On March 8, 9 and 10, 1955, a Fire-Control Symposium was held at M.I.T. by the Servomechanisms Laboratory in joint sponsorship with the Air Force Armament Laboratory, Wright Air Development Center. Representatives of thirty-two interested industrial concerns and nine government agencies attended the symposium. On March ninth the agenda included a description and demonstration of the work done on Problem 126. About 150 participants attended demonstrations of the latest versions of the combined Basic Evaluation and Manual Intervention programs, and some of the other programs of Problem 126. The able and helpful assistance of many Digital Computer Lab personnel is gratefully acknowledged for the success of these demonstrations.

Work is now under way to completely revamp both the Basic and the MIV programs. The basic program is being expanded to include a new additional set of equations and the MIV Program is being redesigned logically and expanded so that more extensive operations will be possible. With the present logic the program demonstrated at the symposium had only five registers unused out of a total of about 3,500 actual program instructions. The new logic will be limited only by the drum capacity of the computer and will be more efficient as well.

Arrangments were made with members of the S and EC group for short term development of several utility programs for use on Problem 126. These routines, some of which have been completed, include a scope routine, a logging and editing routine to give records of all actions taken during a run, and a modified version of the Director Tape program. These routines will be included in the new prototype program and will be described in later quarterly reports.

In preparation for the future re-coding of these programs for the ERA 1103 computer, Problem 256 was initiated by the sponsors of Problem 126 (DIC 7138). A description of the problem and current progress appears elsewhere in this quarterly report.

130 B. N. SIX-COMPONENT DISTILLATIONS, VARIABLE ENTHALPY AND EQUILIBRIUM DATA SIMULTANEOUS NON-LINEAR EQUATIONS

A report on this problem is given in section 2.2 of Part I.

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

This problem has been set aside to account for the WWI time expended in demonstrating the computer to visitors at the Digital Computer Laboratory, in developing routines to be used in these demonstrations, and in testing routines written as part of the training of new staff members.

During the past 3 months, 13 groups visited the Laboratory. The affiliations of some of the larger groups are given in Appendix 2.

A calendar routine was prepared and tested by R. J. Hamlin, MIT Staff member in the School of Industrial Management and E. Raiffa, of the S&EC Group for use in demonstrations. Given any date from March 1,0001 to December 31, 9999, the program calculates and prints on the direct typewriter the day of the week on which it falls. If the given date should fall on a holiday, the name of the holiday will also be printed. In addition, the program calculates the date of Easter Sunday for any given year within the above range.

132 D. SUBROUTINES FOR THE NUMERICALLY CONTROLLED MILLING MACHINE

At present, milling-machine tape-preparation programs for two different types of cams are being developed. One program has apparently been tested successfully and should produce a useful tape during the next run. The program for the other cam is nearing completion. Writing and testing of additional subroutines is continuing.

John Runyon of the MIT Servomechanisms Laboratory is using his study of methods of milling-machine data preparation which included the development of the subroutine library to facilitate the tape-preparation process as research for an Electrical Engineer degree. The thesis is expected to be completed this term.

141. S&EC SUBROUTINE STUDY

Gill's modification of the classical Runge-Kutta fourth-order method of solution of systems of first-order differential equations, described in detail by S. Gill, Proceedings of the Cambridge Philosophical Society, 47 (1950) 96-108, has been coded and put in subroutine form. The subroutine finds the solution at the end of one interval of the system

$$\frac{dy_i}{dx} = f_i(x, y_1, y_2, \ldots, y_n), \qquad 1 = 1\ (1)\ n$$

$$y_i(x_0) \text{ given}$$

$$x_0 \leq x \leq x_0 + h$$

An auxiliary subroutine to evaluate the functions f_i must, of course, be written for each different system.

A subroutine to find a relative minimum of a function f of n variables has been written. The method is to start from an initial estimate x and proceed in the direction of the negative of the gradient for a distance λ. The value λ is also estimated to begin with, and on succeeding iterations is taken as equal to, half, or twice the previous value of λ according as the cosine of the angle between the gradients of corresponding values of f is between 0 and .9, negative, or between .9 and 1. The process continues until successive values of f differ at most by some preassigned ϵ.

A method of economization of power series, by means of Chebyshev polynomials has been coded. The procedure, described more fully (e.g., by C. Lanczos, Tables of Chebyshev Polynomials, NBS Applied

Mathematics Series, no. 9) is briefly as follows: a power series $\sum_{n=0}^{\infty} a_n x^n$ is truncated and then expressed in terms of Chebyshev polynomials:

$$f_N(x) = \sum_{n=0}^{N} \sum_{k=0}^{n} a_n \, t_{nk} \, T_k = \sum_{k=0}^{N} \left(\sum_{n=k}^{N} a_n \, t_{nk} \right) T_k$$

where the coefficients t_{nk} may be found in the NBS publication mentioned above. Now the T_k's may be omitted one by one until the uniform error so made reaches a desired margin. The polynomial approximation may then be rearranged in powers of x again giving in general a short polynomial which approximates the original function more closely than the power series if cut off after the same number of terms.

144 N. SELF-CONSISTENT MOLECULAR ORBITAL

The program represents a mechanization of the Roothaan scheme for solving the many electron self-consistent field problems within the framework of linear combinations of specified functions. The block diagram and details of the program have been given in a previous Summary Report. There is no mathematical guarantee that the procedure should converge and the current difficulty has seemingly arisen from using input data not possessing the proper symmetry properties. It is now felt that the program itself is operating and further work on it has been turned over by Dr. A. J. Meckler to members of the Solid State and Molecular Theory group.

155 N. SYNOPTIC CLIMATOLOGY

The work of the Synoptic Climatology Group of the MIT Meteorology Department over the past quarter has been confined mostly to evaluating cloud seeding experiments. The statistical approach used for the past years by this project was adopted as the method of analysis. It was of interest to determine how much additional information was contained in the circulation pattern regarding precipitation over and above the amount usually accounted for by control and target relationships. The analysis as far as machine computations are concerned has been completed. Evaluation of the results, however, has not been completed.

162 N. DETERMINATION OF PHASE SHIFTS FROM EXPERIMENTAL CROSS-SECTIONS

A phase shift analysis is being made by Dr. F. J. Eppling of the Laboratory of Nuclear Science of the elastic scattering of protons by O^{16} over a range of bombarding energies from about .5 Mev to 4.6 Mev. Cross sections were measured at eight scattering angles from 168.0° to 90.4°. The cross section, $\frac{d\sigma}{dw}$, can be expressed as a function of the scattering angle, θ, and $S^{\pm}$, the non-coulomb phase shift of the partial wave of orbital angular ℓ and total angular momentum $J = \ell \pm 1/2$.

A program has been written by Miss E. Campbell which will find the $S^{\pm}$'s that make the sum of the squares of the errors between the observed and computed $\frac{d\sigma}{dw}$'s a minimum. This program has been designed to work for any number of phase shifts from 2 to 7 and for any energy. As soon as the experimental data has been put into usable form, the program will be run to determine the number of phase shifts and their values required in the energy range mentioned above.

167 B, N. PRODUCTS OF BATCH DISTILLATIONS WITH HOLDUP

A report on this problem is given in section 2.2 of Part I.

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

A report on this problem is given in section 2.2 of Part I.

177 C. LOW ASPECT RATIO FLUTTER

An over-all outline of the problem is given in Summary Report No. 38, Second Quarter, 1954.

At present, work is progressing on collecting the coefficients of the simultaneous equations which will determine the pressure distribution on a flat plate of aspect ratio unity for rigid body translation and pitching.

This involves the multiplication of five complex matrices by five real matrices and the addition of the five resulting matrices. The final complex matrix is an eighteen by eighteen matrix which results in a system of thirty-six real simultaneous equations. Coding for the solution of these equations is now in progress.

This study is being conducted by John R. Martuccelli of the M.I.T. Aero-Elastic and Structures Research Laboratory.

183 D. BLAST RESPONSE OF AIRCRAFT

Since the writing of the last quarterly report, it was found that the Milne's method of numerical integration may cause instability in the solution if the structural discontinuity at buckling is severe. For some parametric values, even an additional iteration cycle could not overcome the difficulty.

As a consequence, the problem was reprogrammed by Y. Shulman of the M.I.T. Aeroelastic and Structures Research Laboratory using the Runge-Kutta method. The two simultaneous second-order equations are written into four simultaneous first-order equations to utilize the subroutine available in the S&EC Group Library. A test run was made for a quasi-steady damping case. The results agree with those obtained by an analytical solution to five significant figures.

The peak responses for a given set of parametric values were computed for 200 cases to examine the effects of various parameters involved in the problem. The lethal criteria for two fictitious airplanes were also established by choosing four values each for altitude, forward velocity, and positive duration of the blast. The machine-computing phase of the problem is now completed.

This work was carried out by H. Lin of the M.I.T. Aeronautical Engineering Department and will be included in his Sc.D. thesis. A modified version of the study is to be published as a U.S.A.F. technical report at a later date.

186 B,L. TRACKING RESPONSE CHARACTERISTICS OF THE HUMAN OPERATOR

This problem seeks to determine the response characteristics of the human operator as a component in a control system. A more detailed description of the problem may be found in Summary Report No. 38. The study is being carried out by J. I. Elkind of the Lincoln Laboratory at M.I.T. The results will be included in his Sc.D. thesis to be submitted to the Electrical Engineering Department.

The Fourier transforms of several more correlation functions of human operator inputs and responses were obtained on WWI. These transforms complete the work to be performed on WWI. The investigation of human operator characteristics continues, however, but the power-density spectra required to determine human operator characteristics will be computed with the aid of some special purpose analogue equipment which has been constructed for this purpose.

189 C. DISTRIBUTION OF GUSTINESS IN THE FREE ATMOSPHERE

The statistics of radar weather echoes are related to the statistics of atmosphere turbulence. (Research Report 22 A and B, Weather Radar Project). The precipitation is here being used as tracers of the motion.

The first probability density of the gustiness is obtained from the transform of the square root of the auto-correlation function. Six such transforms were computed on Whirlwind using a program devised by Douglas Ross under Problem 171 (see Summary Report No. 38). The computations were entirely satisfactory, and for the present no more of these are being contemplated.

193 L. EIGENVALUE PROBLEM FOR PROPAGATION OF ELECTROMAGNETIC WAVES

This problem was described in Summary Report No. 39, July - Sept., 1954. 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.

Program tapes have been made, based on both the power series and the asymptotic series for the Bessel functions. These are being used to give numerical results at three different frequencies. It is expected that enough results will soon be computed to give a comparison with practical measurements that have been made.

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

The program which generates the wave vector groups of vectors of the reciprocal lattice for the body-centered, face-centered and cubic lattices has been written and tested. The program will also generate all wave vectors equivalent to the reduced wave vector for a given set of neighbors in reciprocal space. Only those wave vectors which cannot be carried into one another by operations of the wave vector group are generated. The projection operators for the various irreducible representations of the crystal types named above are also generated on demand of a simply encoded set of numbers. If projection onto an irreducible manifold is desired without regard to a particular basis, the routine will generate that projection operator which leads to the least number of functions in the linear combination which results from the application of the projection operator to the function to be symmetrized.

A program is being written which will take quantities generated by the radial function routine and incorporate them into a tape which will represent in a sense the subspace in which the Hamiltonian matrix is to be diagonalized. This tape is then fed into the matrix diagonalization routine along with the particular symmetry desired and how much of the subspace represented on the tape is to be used. The way this is done is to have the radial wave function routine make a tape which reads into the drum group whose number is the same as that of the band to which the wave functions belong; each successive block on a particular group represents a successive neighbor in reciprocal space. To generate the tape to be read into the matrix routine a tape is read into high speed storage which contains the bands desired, each preceded by a negative number whose magnitude is the order of the neighbor in reciprocal space desired in that band. The input is then a set of coupled numbers.

Production has begun on sodium and the results obtained are being studied by Mr. M. M. Saffren of the Solid State and Molecular Theory Group.

A program to do the method of symmetrized augmented plane waves has been coded and is being tested.

195 C. INTESTINAL MOTILITY

Dr. J. T. Farrar of the Gastroenterological Section of the Evans Memorial Hospital is studying the effect of radiation upon the motility of the small intestine in the rabbit. The analysis of the records is being performed using autocorrelation and Fourier transform, both performed on W.W.I.

During this quarter, twelve autocorrelations have been completed and the results plotted photographically using scope program. Insufficient results are available to draw even tentative conclusions.

It is planned to perform Fourier transform on all autocorrelations. The evaluation of irradiation effect on motility will be based upon differences in: (1) the mean square value, $\overline{(x^2)}$, and (2) relative power contribution of various frequencies as derived from the frequency spectrum.

196. SINGLE ADDRESS COMPUTER

Since the 1953 Summer Session (SS) and SAC programs were written, several changes have been made in the locations of the flip-flops in test storage. In order to avoid the restoration of these flip-flops to their original addresses when SS or SAC problems are run, SS and SAC are being modified to conform to the new addresses of the flip-flops. The corrected SS has been tested and SAC is now being tested.

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 tube, a theoretical investigation of the characteristics of the laminar boundary layer in the entrance region has been carried out by Prof. T. Y. Toong of the Mechanical Engineering Department. Partial differential equations of continuity, momentum, and energy were developed for the laminar boundary layer. These were then transformed into a series of ordinary differential equations, 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 differential equations.

Solution of the third set of the differential equations for the case of constant viscosity and thermal conductivity has been obtained for adiabatic flow at an entrance Mach number of 2.8. However, the convergence of the iteration scheme used to find the correct initial conditions is very slow in this case. Work is being done to improve this situation.

The algebraic program developed by Dr. J. H. Laning in problem 108 has been used in the numerical integration of the three sets of differential equations. Recently, a new program using CS was prepared and run successfully for the solution of the first set of differential equations. The subroutine for the Gill's method was also developed by Dr. Laning. This new program is to be used for the solution of the case of temperature-dependent viscosity and thermal conductivity.

Solutions of the boundary-layer equations for the case of constant viscosity and thermal conductivity are now being prepared for publication in some scientific journal, and as a project report.

201 N. STUDY OF THE AMMONIA MOLECULE

Due to inconsistencies in the original self-consistent field solution, the self-consistent field part of the ammonia molecule calculation has been redone. In addition, the matrix diagonalizations mentioned in the last progress report have been carried out using the secular equation routine, developed by F. J. Corbato under problem 172, and the ground state energies of the Ammonia molecule have been calculated. The analysis of the solutions is now being carried out by Prof. Harvey Kaplan at the University of Buffalo. This work was carried along by members of the M.I.T. Solid State and Molecular Theory Group.

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

A report on this problem is given in section 2.2. of part I.

204 N. EXCHANGE INTEGRALS BETWEEN REAL SLATER ORBITALS

This problem is being studied by members of the Laboratory of Molecular Spectra and Structure of the University of Chicago in cooperation with the MIT Solid State and Molecular Theory Group. A routine was developed by P. Merryman of the Chicago group for evaluating two-center exchange integrals. A more detailed discussion of this routine was given in Summary Report No. 39. The routine is still being tested.

211 C. SERVO RESPONSE TO A COSINE PULSE

A description of the original problem may be found in Summary Report No. 39 for the Third Quarter, 1954. In Summary Report No. 40 there is a terminating report for the original problem under this number as well as a description of a related problem. During the past quarter, some work was done on the related problem, described as follows.

It is desired to find numerically the maximum response s(t) for some parameter pairs (ζ, T_p/T_n), $0.01 \leq \zeta \leq 5$, $0.1 \leq T_p/T_n \leq 10$ in the equation

$$(1/\omega_n^2)\,\ddot{x} + (2\zeta/\omega_n)\,\dot{x} + x = G(t), \text{ where}$$

$$T_n = 2\pi/\omega_n,\ \dot{x} = dx/dt,\ \ddot{x} = d^2x/dt^2,$$

$$G(t) = 1/2\left[1 - \cos(2\pi t/T_p) + 2\zeta(T_n/T_p)\sin(2\pi t/T_p)\right],$$

$$\text{for } 0 \leq t \leq T_p,$$

and $G(t) = 0$ for $t > T_p$.

Coding of the problem using CS II was accomplished by Dr. J. M. Stark of the M.I.T. Instrumentation Laboratory. For application of the results obtained, reference is made to pp. 704, 705 of INSTRUMENT ENGINEERING, Volume II, by Draper, McKay, and Lees, and to Volume III (yet to appear) of the same work.

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

The program for calculating dispersion curves of surface seismic waves on multi-layered media is operating satisfactorily. As mentioned in Summary Report No. 40, the program was written to handle a five-layered medium. However, by resetting one constant, as many layers as desired can be handled. On the average, one data point for a five layer case requires approximately 1.5 minutes. Reducing or increasing the number of layers gives a corresponding reduction or increase in computing time of, roughly, 1/4 seconds per layer.

This method is merely a solution for the roots of an algebraic equation, the lowest of which correspond to Rayleigh mode propagation. It has been used with no modification to solve for the large roots corresponding to normal modes of propagation. The method requires two initial estimates of the phase velocity at each value of wave number for which a phase velocity is sought and the final solution is the root nearest to the first estimates. Thus a Rayleigh or a normal mode velocity will be obtained depending on which is closer to the estimates.

The program has been checked with dispersion curves in literature and is being used to calculate new results. It has been decided not to calculate group velocity curves since machine time would be better expended on phase velocities.

An interesting, but time-consuming, possible application was brought up in a discussion of the problem with the head of the Lamont Geological Observatory at Columbia University. It is believed that many unexplained results of seismic measurements at sea are due to smooth changes in velocity and density with depth. This situation might be approximated by a large number of layers with small changes between each.

This work is being carried out by K. Vozoff of the MIT Geology and Geophysics Group as part of the requirements for a Ph.D. thesis.

215 B. DYNAMIC BEHAVIOR OF INDUSTRIAL PROCESSES

The application of automatic control to industrial processes would be greatly facilitated if the dynamic behavior of the process could be determined from measurements made during normal operation of the process, without shutting the process down or introducing inputs of a transient or periodic nature. An experimental measurement of the impulse response of a linear heat transfer system subject only to random disturbances of its operating point has been carried out in the Process Control Laboratory with the cooperation of Professors D. P. Campbell and L. A. Gould. Input auto-correlation functions and input-output cross-correlation functions were computed using programs developed under problem 107 by D. T. Ross. The frequency response computed from the results of the correlation study agrees well with that measured on the same system by conventional techniques.

A method which avoids the necessity of solving an integral equation to find the impulse response from the correlation functions is described in a forthcoming R.L.E. Progress Report, covering the period December 1st to Feb. 28, 1955. An autocorrelation and Fourier transform required by this method have been carried out using Ross's programs, but I.B.M. equipment will be used for the less massive computations which remain to be done.

The results of this experimental work have shown that general purpose digital machines, such as Whirlwind I, as well as business machines of the I.B.M. type, are much more suitable for computing the correlation functions required in the study of industrial processes than are special-purpose analog correlators. The digital machines offer higher accuracy than the analog machines, and are free of limitations of available delay-time and frequency range.

This work was carried out by S. Margolis of the Statistical Communication Theory Group of R.L.E. under the supervision of Professor Y. W. Lee.

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

A report on this problem is given in section 2.2 of Part I.

218 N. TRANSFORMATION OF INTEGRALS FOR DIATOMIC MOLECULES

A discussion of this problem has been included by Dr. Nesbet in his report on Problem 234.

219. COMPARISON OF SIMPLEX AND RELAXATION METHODS IN LINEAR PROGRAMMING

A program has been written and checked for the solution of simultaneous equations by a method of cyclic projections. If $Ax \leq b$, A an m x n matrix, and X_i is an approximate solution, a better solution, X_{i+1}, is obtained from

$$X_{i+1} = X_i - \frac{\bar{r} \cdot e_{i \bmod m}}{(A^T e_{i \bmod m})^2} \quad A^T e_{i \bmod m}$$

where e_K $(0 \leq K \leq m-1)$ is the vector with $(K+1)^{th}$ component 1 and all other components 0, and

$$\bar{r}_i = \max(r_i, 0), \; Ax_i - b = r_i$$

In spite of the computational speed of this technique, the convergence is so slow as to render it impractical. Various methods of accelerating the convergence have been proposed and are under consideration.

A program for the solution of linear programming problems by a method similar to one proposed by Cooper, Charnes, and Henderson (An Introduction to Linear Programming, J. Wiley and Sons, New York, 1954) has been written and is being checked. Other methods will be compared with this technique.

This problem is being carried out by Mr. Dean N. Arden and Mr. Elliot Raiffa of the Digital Computer Laboratory Staff.

221 B. COURSE 6.25, MIT

Sixty-one students enrolled in course 6.25, MACHINE-AIDED ANALYSIS, given first semester, 1954, by the Electrical Engineering Department. The course was jointly given by Profs. W. K. Linvill, R. C. Booton, and C. W. Adams. Computational techniques of analog and digital computers, the solution of engineering problems by numerical methods, and numerical analysis were studied during this course.

TAC, the summer session Three Address Computer, was used by the students for the solution of the following problem:

Consider the Van der Pol equations

$$\ddot{y} + \epsilon(y^2 - 1)\,\dot{y} + y = 0, \text{ where}$$
$$\dot{y}(0) = a$$
$$y(0) = b$$

For this equation, assumed values of ϵ, a, and b are chosen so that $\ddot{y}_{max} < 10$, $\dot{y}_{max} < 10$, and $y_{max} < 10$. Solve the equation using intervals, $h = 0.1$. Print out the values of y for integer values of t and carry out the solution until the value of y has passed its second positive peak. Scale factor the solution so that all of TAC's 8 digits are used. Use the rectangular rule of integration.

Each student programmed and prepared on punched tape his own program. Each solution took approximately 3 minutes of WWI computer time and a total of 37 minutes was used by this problem during this report period.

222 C. HELICOPTER ROTOR STABILITY

The transient response in the flapping of a helicopter rotor blade has been calculated by Y. Shulman of the MIT Aeroelastic and Structures Research Laboratory. These calculations involved the integration, using the fourth-order Runge-Kutta method, of two ordinary, linear second-order differential equations with variable coefficients. One purpose of these calculations was to check the results obtained by an approximate analytical solution to this problem which was dealt with by Y. Shulman in his Master's Thesis*. The other purpose was to compare results obtained by assuming the blade to be flexible in bending to those for rigid blades and check with experimental results.

Calculations were carried out for a variety of blade mass constants and over a wide range of forward speeds.

The results have shown conclusively that within the limits of the approximations, blade flexibility affects the stability regions of the motion considerably. The results of the analysis which include blade flexibility tend towards better agreement with experimental results. The results of the analytical solution are unconservative.

A full description of the problem, and the results of these calculations were included in a paper delivered by Y. Shulman at the 23rd annual meeting of the Institute of Aeronautical Sciences, January 27, 1955**.

223 B, N. INVESTIGATION OF TURBULENT FLOW

This project is sponsored by the Office of Naval Research under contract No. N5-ori-07874. It deals with the investigation of turbulent velocity fluctuations in open channel flow by means of a Pitot tube-pressure cell combination. In previous summary reports, this problem was described under problem 107.

During the interim, the phase of this investigation concerning the measurement of some turbulence characteristics in the wake of a circular cylinder in supercritical open channel flow was completed. Auto-correlation curves were obtained from the Digital Computer Laboratory for points near the centerline of the wake at three stations 40, 50, and 70 diameters downstream from the test body. From these curves, by the process explained in Summary Report No. 40 under problem 107, the scale of macro-turbulence or the mean eddy size was computed. The variation of this parameter with distance downstream gives an indication of the type of turbulent decay present in the wake. The values computed showed an increase with the square root of the distance downstream from the cylinder. This indicates that the rate at which the smaller eddies in the flow are decaying into heat must be greater than that at which the larger ones are breaking up. This same type of variation has been observed by investigators in the wake of a grid and is indicative of the isotropic nature of the turbulence present in the core of the wake.

Additional runs are planned by F. Raichlen of the MIT Hydrodynamics Laboratory for the near future to ascertain the applicability of a piezoelectric ceramic transducer with impact tube attachment to the turbulence problem.

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

This problem was prepared for computation by Geirmundur Arnason and is being programmed by William Wolf. The results will be analyzed by the Pressure Change Project under the supervision of Professor James M. Austin of the MIT Meteorology Department.

The rising and sinking air motion causes the weather to change from clear skies to rain and vice versa. This important vertical motion cannot be measured directly so that the meteorologist must estimate the vertical velocity by observing its effect on other measurable quantities, such as temperature. To date our information on the field of vertical motion is very inadequate. It is the objective of the proposed set of computations to determine this field for a series of weather situations. The results should contribute to basic knowledge

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* Shulman, Y., "Stability of a Flexible Helicopter Rotor Blade in Forward Flight", S. M. Thesis, Aeronautical Engineering Department, Massachusetts Institute of Technology, June 1954.

** Shulman, Y., "Stability of a Flexible Helicopter Rotor Blade in Forward Flight', preprint No. 521, IAS, January 1955.

concerning the behavior of the atmosphere. Furthermore, they should greatly aid the continuing research in the field of numerical weather prediction. Various modified forms of the equation for the change in the vertical component of vorticity are utilized to predict tomorrow's flow pattern. A lack of knowledge of the relative importance of the vertical motion terms in the vorticity equation is hampering the research in the field of numerical weather prediction.

The main problem is to determine the three-dimensional fields of vertical velocity (and horizontal divergence) by means of the observed pressure field. For this purpose the adiabatic equation is integrated between the two pressures $p = p_1$ and $p = p_2$ $(p_1 > p_2)$.

$$\frac{\partial}{\partial t}(Z_2 - Z_1) + \frac{R}{g}\int_{\log p_2}^{\log p_1} V \cdot \nabla T \; d\log p + \frac{R \cdot S}{g}\int_{\log p_2}^{\log p_1} W \, d\log p = 0 \qquad (1)$$

Moreover the horizontal divergence is determined from the continuity equation

$$\operatorname{div} V = W + \frac{\partial W}{\partial \log p} \qquad (2)$$

where Z_1 and Z_2 are the heights of the pressure surfaces p_1 and p_2 respectively, R is the gas constant for dry air, g the acceleration of gravity, V the geostrophic wind, T the temperature, ∇T the horizontal nabla operator, S the static stability, and W the vertical velocity defined as

$$W = -\frac{d \log p}{dt} \qquad (3)$$

where $\frac{d}{dt}$ is the total time derivative and $\frac{\partial}{\partial t}$ the local time derivative.

Observed Z's for p = 1000, 850, 700, 500, 300, 200, and 100 mb are available 12 hours apart in time. The first term in (1) is replaced by a 12-hour change in Z and interpreted as a local time derivative at the midpoint of the time interval. The geostrophic wind V is related to the height Z by the equation

$$V = \frac{g}{f} K \times \nabla Z \qquad (4)$$

where f is the Coriolis parameter and K a unit vector directed upwards.

Observed temperatures are not available, but an approximate temperature field can be derived from the heights (the Z-field). This is done in part I of the program. Since both V and ∇T are thus known, the second term in (1) can be evaluated. The third term in equation (1) contains the only unknown quantity W, since the static stability S is derived from the Z-distribution (part I of the program). Nothing is known about the W-distribution except that W = 0 at p = 1000 mb. An approximate vertical distribution of W is obtained by overlapping second order polynomials in $\log \frac{p_1}{p}$ of the form

$$W = W_1 + \log\left(\frac{p_1}{p}\right) a(x,y) + \left[\log\left(\frac{p_1}{p}\right)\right]^2 b(x,y) \qquad (5)$$

where a(x,y) and b(x,y) are two parameters to be determined from observations, x and y are the horizontal coordinates, W_1 is the vertical velocity at $p = p_1$ and W the vertical velocity at a variable p. We now put p_1 = 1000 and p_2 = 700 mb and carry out the integration of (1) utilizing the boundary condition W = 0 at p_1 = 1000 mb. The resulting equation contains the two unknown a(x,y) and b(x,y). An additional equation is obtained by putting p_1 = 700 and p_2 = 500 mb and integrating (1). We have now two equations with two unknowns and these are solved by conventional methods. Upon determination of a(x,y) and b(x,y) the vertical velocity at 700 mb is obtained from equation (5). Starting anew with p_1 = 700 mb and $W_1 = W_{700}$ known, the procedure is repeated (p_2 = 500 and 300 mb respectively) and a new set of parameters is determined. Altogether four sets a, b are computed and the vertical velocity profile is composed of four overlapping parabolas with horizontal axis, see equation (5).

The field of horizontal divergence is readily computed from equation (2).

Part II of the program deals with the computation of the quantities W and div V. The fields of vertical velocity and horizontal divergence being known besides the original Z - field, all the terms in the vorticity equation

$$\frac{\partial \eta}{\partial t} + V \cdot \nabla \eta - W \frac{\partial \eta}{\partial \log p} + \eta \operatorname{div} V - \nabla W x \frac{\partial V}{\partial \log p} \cdot K = 0 \tag{6}$$

can be computed. Here $\eta = \frac{g}{\rho} \nabla^2 Z + f$ is the absolute vorticity, f the Coriolis parameter, and ∇^2 the horizontal Laplace operator. Due to insufficient knowledge of the fields of vertical velocity and horizontal divergence, the three last terms have frequently been neglected in the applications of equation (6).

The third and the last part of the program deals with the computations of the various terms in (6) and gives a simple statistical measure for the relative orders of magnitude.

The programming of the problem is nearing completion. The program cycles through without alarms but not all of the answers are correct at present. It is expected that the conclusive checkout will be completed at the beginning of the next quarter.

An interesting facet of the programming is the use of the symbol generator* as an output device. This special mode of scope output displays a coded combination of seven lines comprising a rectangular figure eight in approximately twice the time it takes to display a point. The usual type of number display being a coded combination of an 3 by 5 array of points, the use of the symbol generator effectively reduces the machine time by a factor of four.

The coding employs the WW1 order code exclusively since the four significant digits required may be carried in a WW1 word. Where averages are performed a routine for combining the major and minor parts of a double length register number is used which is similar to that used in the Programmed Arithmetic routine.

A general, yet concise subroutine for treating the Auxiliary Drum as a continuous storage medium was written. This was necessary since all of the available Auxiliary Drum storage (with the exception of about 200 registers) is used during the course of the program.

225 B,N. NEUTRON-DEUTERON SCATTERING.

A report on this problem is given in section 2.2 of Part I.

228 N. EVALUATION OF DIFFERENCE DIFFUSION EQUATION

A report on this problem is given in section 2.2 of Part I.

230 C. DYNAMIC ANALYSIS OF BRIDGES

Saul Namyet of the MIT Civil and Sanitary Engineering Department is determining the dynamic response of various types of simple span bridge structures. The purpose of the project is to determine the minimum value of a parameter q that is required to cause a predetermined maximum response. The parameter q defines the forcing function for any orientation of the impulsive load to the bridge.

For purposes of this investigation, a bridge is represented dynamically by a single-degree-of-freedom system consisting of a concentrated mass and a spring, having various resistance-deflection characteristics.

The solution is achieved by application of the second difference equation

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

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*For a detailed description see M-1623-2 "Programming for In-Out Units".

to the differential equation

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

where

$\ddot{x}(t_n)$ = acceleration at time (t_n)

P_n = force applied at time (t_n)

R_n = resistance developed in spring at time (t_n)

The overall program is advancing satisfactorily along the lines reported previously.

231 B,N. REACTOR RUNAWAY PREVENTION

A report on this problem is given in section 2.2 of Part I.

232 B. ENERGY LEVELS IN A SPHEROIDAL SQUARE WELL

The problem being studied by K. Gottfried of the Laboratory for Nuclear Science is an investigation of Bohr and Mattelson's Model of Nuclei. A first step in such an analysis is the computation of wave functions and energy levels for nucleons moving in a deformed potential. The investigation of this first step[1] (which is described in Summary Report No. 40) is virtually completed, and a final report will be submitted in the next Quarterly.

233 C. UTILITY STOCK PRICES

This project, which involves statistical regression analysis of utility stock prices, is being conducted by D. Durand of the School of Industrial Management with two distinct goals in mind. In the first place, it is an experiment in applying regression analysis to financial problems in order to (1) develop better methods of ascertaining the cost of equity capital and (2) to establish principles applicable to corporate financial management and to security analysis. In the second place, it is an experiment in reducing the arduous computing labor heretofore encountered in regression analysis to practical proportions by the specific means of a modern, tape-fed electronic computer.

The problem entails a series of computations that can be classified into four groups, as follows:

1. Preliminary processing of data.
2. Summation of squares and products - $\sum x_i^2$ and $\sum x_i x_j$
3. Solution of simultaneous linear equations with concurrent operations required in statistical regression analysis.
4. Final processing.

Of these, the nature of 1. and 4. is not yet decided. Possibly all or part of the operations required can be performed by hand or with desk calculators. One preliminary operation that is not well suited for hand work is the conversion of some five to ten thousand decimal numbers into logarithms. Group 2 is laborious for desk calculation but conceptually simple; a subroutine for doing this work on WWI may easily be set up. Group 3 presents the real challenge.

Although the literature on solving simultaneous equations is voluminous, there appears to be room for considerable development work. In statistical regression, it is necessary to solve the so-called normal equations, which could be done by any of the already developed methods, but the problem does not end here. In addition, residual variances and standard errors have to be calculated. Although these additional operations

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[1] See also K. Gottfried and V. F. Weisskopf, Quarterly Progress Report, L.N.S., February 1955

can be treated separately after the solution of the normal equations, they can also be incorporated directly into the solution of the normal equations. The scientific contribution, if any, will come from the effective integration of a number of computation steps into a single systematic routine.

Progress to date has consisted in writing an experimental program, which is now in the process of being tested. At the same time we are thinking about possible improvements in this program that will make it more general and extend its usefulness to a wider class of problems.

234 N. ATOMIC INTEGRALS

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 calculation 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-confistent 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 function. 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 elsewhere.[1]

The program for atomic integrals reads in a list of parameters (ℓ_a, A, Z_a), specifying a set of Slater orbitals

$$\eta_a = r^{A+\ell_a} e^{-Z_a r} Y^m_{\ell_a} (\theta, \phi),$$

and prints out all independent one-and two-electron integrals (overlap, kinetic energy, and Coulomb potential energy), for normalized η's. The normalization constants are also printed out. Here A and ℓ_a are any non-negative integers and Z_a is any positive number.

The transformation of integrals required in Stage B is essentially the same in both atomic and molecular problems. A two-electron integral $[ij|k\ell]$, in Mulliken's notation, is invariant under interchange of indices i and j or of k and ℓ, or of the index pairs (ij) and ($k\ell$). Given the expansion coefficient $X_{\alpha i}$ of

$$\phi_\alpha = \sum_i X_{\alpha i} \eta_i,$$

the transformation required for two-electron integrals is

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[1] R. K. Nesbet, Quarterly Progress Report, Solid State and Molecular Theory Group, MIT, April 1955

$$[\alpha\beta|\gamma\delta] = \sum_i \sum_j \sum_k \sum_\ell X_{\alpha i} X_{\beta j} X_{\gamma k} X_{\delta \ell} [ij|k\ell].$$

All functions and coefficients are assumed to be real. The corresponding transformation on two indices for one-electron integrals is considerably more manageable.

The Whirlwind program for this transformation constructs all independent elements $[\alpha\beta|\gamma\delta]$ from $[ij|k\ell]$ without repeating equivalent calculations. The symmetries of this four-index form under interchange of the indices as well as any symmetry properties of the basic orbitals (due to spatial symmetry of the Hamiltonian) are taken into account to reduce the number of arithmetic operations in this transformation as much as possible.

235 B,N. EIGENVALUES FOR A SPHEROIDAL SQUARE WELL

A report on this problem is given in section 2.2 of Part I.

236 C. TRANSIENT RESPONSE OF AIRCRAFT STRUCTURES TO AERODYNAMIC HEATING

The study of transient response of aircraft structures to aerodynamic heating was initiated on January 3, 1955 by L. A. Schmit of the MIT Aero-elastic and Structures Research Laboratory. H. Parechanian has been responsible for a major portion of the programming during the latter half of this report period.

The overall problem is that of investigating the influence of aerodynamic heating on the structural design of high speed aircraft. One important step in the solution of the overall problem is to determine the transient temperature distributions in built-up aircraft structure. This first phase requires the solution in generalized form of two idealized heat flow problems. The first of these two idealized heat flow problems (Problem I) has been formulated and solved.

Problem I is that of determining the transient temperature response of a thin plate exposed to a timewise step function change in adiabatic wall temperature with a turbulent boundary layer type chordwise variation of the heat transfer coefficient.

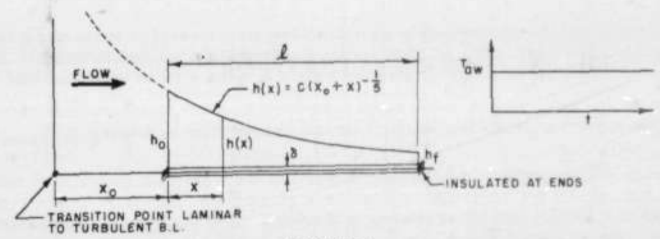

FIGURE I

SCHEMATIC REPRESENTATION OF PROBLEM I

The problem is formulated in terms of the following symbols.

T_{aw} = adiabatic wall temperature

$h(x)$ = heat transfer coefficient at x

ℓ = plate length

δ = plate thickness

h_o = heat transfer coefficient at $x = 0$

x = location along plate referred to leading edge of plate considered

t = time

T = Temperature

ρ = weight density of plate material

k = thermal conductivity of plate material

C_p = specific heat of plate material

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

If it is assumed that h(x) is not a function of t or T, and the thermal properties of the plate are constant, the heat balance equation for the plate shown in Figure 1 is as follows:

$$h(x)\ (T_{aw} - T) + k\,\delta\,\frac{d^2T}{dx^2} = \rho\, C_p\, \delta\, \frac{dT}{dt} \tag{1}$$

The intitial and boundary conditions are assumed to be as follows:

$$T = T_i \text{ when } t = 0 \tag{2}$$

$$\frac{dT}{dx} = 0 \text{ at } x = 0 \text{ and } x = \ell \tag{3}$$

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

$$\phi = \frac{T_{aw} - T}{T_{aw} - T_i} \ ; \quad \bar{x} = \frac{x}{\ell} \ ; \quad \bar{t} = \frac{h_o}{\rho\, C_p\, \delta}\, t$$

and

$$f(\bar{x}) = \frac{h(\bar{x})}{h_o} \ ; \quad f(1) = \frac{h_\ell}{h_o} \ ; \quad \beta = \frac{k\,\delta}{h_o \ell^2} \ .$$

With the notation above, the problem is stated in nondimensional form as follows:

$$\frac{d\phi}{d\bar{t}} + f(\bar{x})\phi = \beta\, \frac{d^2\phi}{d\bar{x}^2} \tag{1a}$$

$$\phi = 1 \text{ when } \bar{t} = 0 \tag{2a}$$

$$\frac{d\phi}{d\bar{x}} = 0 \text{ when } \bar{x} = 0 \text{ and } \bar{x} = 1 \tag{3a}$$

If the plate length ℓ is divided into n geometric elements of length $\Delta \bar{x} = \frac{1}{n}$, and it is understood that i refers to the i^{th} physical element, and j refers to the j^{th} time increment, then the uncoupled forward finite difference formulation can be written as follows:

$$\phi_{1,j} = \left[1 - f_1(\bar{x})\, \Delta\bar{t} - \frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\right] \phi_{1,\,j-1} + \frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\, \phi_{2,\,j-1} \tag{4}$$

$$\phi_{i,j} = \frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\, \phi_{i-1,j-1} + \left[1 - f_i(\bar{x})\Delta\bar{t} - 2\,\frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\right] \phi_{i,j-1} + \frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\, \phi_{i+1,j-1} \tag{5}$$

$$\phi_{n,j} = \frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\, \phi_{n-1,j-1} + \left[1 - f_n(\bar{x})\Delta\bar{t} - \frac{\Delta\bar{t}\,\beta}{(\Delta\bar{x})^2}\right] \phi_{n,j-1} \tag{6}$$

or in matrix form

$$\{\phi_j\} = [C]\, \{\phi_{j-1}\} \tag{7}$$

with the initial condition $\{\phi_o\} = \{1\}$

The final production program is based on a fifteen element physical grid (n=15). Given numerical values for the parameters β and f(1) as well as a value of $\Delta\bar{t}$ the program computes the coefficients that make up the matrix $[C]$ in eq. 7 using CS II. Since it can be seen from the formulation that all non-zero terms in the matrix $[C]$ are between zero and one the results of the CS II calculations are stored as single length WWI numbers. The evaluation of $\{\phi_j\}$ is then carried out according to eq. 7 in WWI. Since the bulk of the calculation consists of performing the matrix multiplication indicated in eq. 7 the time saving that results from performing this part of the program in WWI rather than CS II is substantial (at least four times faster).

The output display is controlled by the nondimensional temperature response $(1-\phi_{1,j})$ of the leading edge element. As $(1-\phi_{1,j})$ reaches 0.1, 0.2, . . . etc. up to 0.9 at intervals of 0.1, the fifteen element nondimensional temperature distribution is stored as well as the time ($\bar{t} = j\Delta\bar{t}$) associated with it. When $(1-\phi_{1,j})$ exceeds 0.9 the stored results for the case (f(1), β) just completed are displayed. On the first scope frame, $1-\phi_{i,j}$ versus $\bar{x}$ for various $\bar{t}$ are plotted. The first frame is essentially a family of nine nondimensional temperature distribution curves. On the second scope frame $1-\phi_{i,j}$ versus $\bar{t}$ for various $\bar{x}$ are plotted. The second frame is essentially a family of fifteen nondimensional temperature time history curves. The nine pertinent times are typed out via magnetic tape. The final values of $\phi_{i,j}$ are also typed out via magnetic tape and would serve as an initial condition in the event that it ever became necessary to carry the calculation nearer to the steady state condition.

The selection of $\Delta\bar{t}$ in order to prevent divergent oscillation of the difference solution is a routine matter. (Ref. F. B. Hildebrand, Methods of Applied Mathematics, Prentice Hall, Inc., New York, 1952, pp. 323-345.) The maximum value of $\Delta\bar{t}$ that may be used for a given β in the fifteen element program is given by eq. 8.

$$\Delta\bar{t}_{max} = \frac{1}{450\beta + 1} \tag{8}$$

It was found by trial that satisfactory damping of the convergent oscillations, characteristic of the finite difference solution at early times, could be insured by selecting $\Delta\bar{t}$ such that approximately four hundred time cycles are required for the nondimensional temperature of the leading edge element $(1-\phi_{1,j})$ to reach 0.9 of its steady state value which is 1.0.

The convergence of the fifteen element solution was examined by writing a forty-five element program and running cases at the limits of the β and f(1) parameter ranges. It was found that the maximum difference between the fifteen and forty-five element response occurred when f(1) was a minimum and β was a maximum. (f(1) = 0.1, $\beta = 5 \times 10^{-2}$). As a result of the calculations made employing the forty-five element program it was decided that the fifteen element program yielded results satisfactory for the purposes of the present work.

During the course of the work just discussed it became apparent that for certain values of β and f(1) satisfactory results could be obtained by neglecting chordwise conduction. The nondimensional temperature response is obtained in simple closed form if chordwise conduction is neglected.

$$\frac{d\phi}{d\bar{t}} + f(\bar{x})\phi = 0\,, \quad \phi = 1 \text{ when } \bar{t} = 0 \tag{9}$$

Hence,

$$\phi = e^{-f(\bar{x})\,\bar{t}} \tag{10}$$

Because of this fact the program has been augmented. For each case $(f(1), \beta)$ there are 135 values of $\phi_{i,j}$ in storage just prior to entering the output display portion of the program. The augmented program computes the 135 corresponding values of $\phi_{i,j}$, when conduction is neglected, according to eq. 10, then computes and prints out via magnetic tape 135 values of e, where e is determined as follows:

$$e = \frac{\phi_{i,j} - (\phi_{i,j})_{\text{conduction neglected}}}{1 - \phi_{i,j}} \tag{11}$$

As a result of running 32 cases employing the augmented program the following tentative conclusion has been reached. If $\beta < 5 \times 10^{-2}$ and $0.1 < f(1) < 1.0$, less than 5% difference in the nondimensional temperature response results from neglecting chordwise conduction provided

$$f(1) > 0.45716 \log \beta + 1.42247 \tag{12}$$

Work on Problem I is essentially complete. It is intended to program Problem II, the web-plate temperature response problem, during the next report period. Formulation and discussion of the results obtained for Problem II will be presented in the next report.

237 C. AUTOCORRELATION FUNCTION OF SUBMITTED DATA

This problem was concerned with finding the autocorrelation function of data derived from work originating at the Instrumentation Laboratory at M.I.T. The problem used the subroutine developed by Douglas Ross for computing autocorrelations in problem 107. The autocorrelation function was derived and the problem was completed.

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

A report on this problem is given in section 2.2 of Part I.

239 C. GUIDANCE AND CONTROL

This problem encompasses a variety of calculations relating to the guidance and control of aircraft. Details are for the most part classified. However, as incidental by-products of this investigation, standard subroutine library tapes have been prepared for:

1) the solution of an arbitrary number of ordinary first order differential equations using the method of Gill;
2) the minimization of an arbitrary function of n variables by the method of steepest descents.

Further discussion of these subroutines may be found under problem 141.

This investigation is being carried out under the supervision of Dr. J. H. Laning, Jr., of the Instrumentation Laboratory.

241 B,N. TRANSIENTS IN DISTILLATION COLUMNS

In the past three years the availability of the Whirlwind Computer for thesis work has been used by members of the Chemical Engineering Department at M.I.T. to study several problems in distillation which are too complicated to solve by ordinary methods. Up to the present, work has been done by Jack O'Donnell on the solution of some complicated multicomponent problems and on batch distillation problems, and some work has been done by Smith, Polk, and Jordan on unsteady state continuous distillation systems.

All of the work on unsteady-state problems has been on an ideal system which satisfies the following conditions:

1) A two-component system.
2) Constant molal overflow above and below the feed plate.
3) Equilibrium condition between the liquid and vapor phases represented by $y = \frac{\alpha x}{1+(\alpha-1)x}$ where x and y are the mole fractions of the more volatile component in the liquid and vapor phases respectively. Furthermore α is assumed to be constant throughout the column.
4) Average composition of the liquid leaving each plate equal to the composition of the liquid on the plate.
5) Average composition of the vapor leaving each plate given by the equilibrium condition with the liquid on the plate.
6) Holdup of all the plates constant with time and equal for all plates.
7) Holdup of condenser and reboiler negligible.
8) Feed introduced into column as a saturated liquid.

The operation of such a system can be described by a set of non-linear, first-order differential equations. Such a set of equations can be solved by any of a number of different types of finite-difference approximations to almost any desired accuracy. The Runge-Kutta approximations have advantages which make them the easiest to use with a large scale digital computer. It has been found that by using a second-order Runge-Kutta approximation with an interval size equal to 0.1 units of liquid throughput (time x liquid flowrate/individual plate holdup) insures convergence and at least 0.05% accuracy for nearly all problems of this type.

Programs have been written for the CS II computer for a distillation column containing up to fifty plates in which any one or more of the following variables have undergone a sudden change:

1) Feed composition
2) Reflux ratio
3) Vapor rate

It is proposed to study how a column will react to such sudden changes and to attempt correlations for the length of time that it takes a column to approach its new equilibrium condition. It is also proposed to write programs for and to study a column in which some variable is controlled to offset the effects of a change in some other variable. For example the reflux ratio might be controlled while the feed composition undergoes a change so the tops composition remains approximately constant.

Finally it is proposed to write programs for and to study more complicated unsteady-state distillation problems in which one or more of the above eight conditions are relaxed.

These studies will bc carried out by S. H. Davis, Jr. of the Chemical Engineering Department.

242 N. NUMBER OF STRUCTURES OF RELATIONS ON FINITE SET

A report on this problem is given in section 2.2 of Part I.

243 D. CRYSTAL FILTERS

The data obtained from this problem is designed to provide a simple approximate solution to a phase of the design of filters using quartz crystals as elements. The part done on WWI consisted of the systematic computation of products, using cycle counters, with the results being obtained on film. There are no plans for any further work to be done on WWI. The problem was done for David Kosowsky and will be published in his Ph.D. thesis and in the Research Laboratory for Electronics Technical Report. Hannah Paul was the programmer.

244 C. DATA REDUCTION FOR X-1 FIRE CONTROL

This problem is concerned with computing from fire control signals how far fictitious projectiles miss an observed target. Because of the large amount of data taken for each target run, use is made of the great storage capacity of the auxiliary drum. The main tape for this problem calls data off the drum and into high speed storage, a block at a time, for each cycle of computation.

Calculations where accuracy is a factor, in general, are carried out with programmed arithmetic, whereas some searching procedures are coded in the basic code of WWI. Extensive ballistic data also is stored on the auxiliary drum. Register numbers for needed ballistic data are computed in the basic code of WWI.

A number of shorter tapes prepared for this problem are concerned with analyzing system errors and finding suitable corrections to apply to dial readings for the raw data used with the main tape.

This work is being carried out by Dr. J. M. Stark of the M.I.T. Instrumentation Laboratory.

245 N. THEORY OF NEUTRON REACTIONS

Recent treatments of the theory of nuclear reactions have shown that as far as neutron reactions are concerned, the gross aspects of the problem could be explained by assuming that the neutron moves in a complex potential. In the first treatment of this problem it was assumed that the potential was in the form of a rectangular well. This led to relatively good agreement with the total cross-sections and to only rough agreement with the inelastic scattering and angular distribution of elastically scattered neutrons. The qualitative agreement here, however, has encouraged us to go on. It was felt that a potential well which was not as idealized as the square well, in particular a well which had a tail to it, would bring the experiment and the theory into closer agreement.

Preliminary analytical work has indicated that a well of the following form should be close to the correct description

$$V = -V_o(1+i\zeta)\left[1 - \tanh\frac{r - R}{d}\right].$$

The parameters describing the well are

V_o = the depth of the well

R = the approximate radius of the nucleus

d = the rate at which the square well falls off to zero

ζ = a measure of absorption inside the nucleus

The use of this well has been encouraged by a later work of Saxon and Woods in which it was found that a well of this kind would simulate the results of experiments with 18 mev protons. The problem was transformed into a nondimensional form by introducing the parameters

$$K_o^{\ 2} = \frac{2m}{\hbar^2} V_o R^2, \quad \delta = d/R, \text{ and } x = kR$$

where m = mass of neutron and $k^2 = 2m/\hbar^2 E$ where E is the neutron energy.

It is desired to calculate the predicted scattering for a variety of values of these parameters to pick out the best values of δ and ζ so as to give the best agreement with data.

The radial equation to be solved for the ℓ^{th} partial wave is

$$u_\ell'' + \left\{1 - \frac{\ell(\ell+1)}{y^2} + V(y)\right\} u_\ell = 0 \qquad u_\ell(0) = 0$$

where the potential

$$V(y) = 1/2\,\frac{X_o^{\ 2}}{x^2}\,(1+i\zeta)\left(1-\tanh\frac{y-x}{x\delta}\right)$$

From u_ℓ, the phase shift δ_ℓ can be found by the equation

$$\cot\delta_\ell = \frac{\int_0^\infty y\, n(y)\, V(u)\, u_\ell\, dy - 1.3\cdots(2\ell+1)\left(\frac{u_\ell}{y^{\ell+1}}\right)_{y=0}}{\int_0^\infty y\, j_\ell(y)\, V(y)\, u_\ell\, dy}$$

From $\cot\delta_\ell$ can be found

$$\eta_\ell = e^{2i\delta_\ell} = \frac{\cot^2\delta_\ell - 1}{\cot^2\delta_\ell + 1} + 2i\,\frac{\cot\delta_\ell}{\cot^2\delta_\ell + 1}$$

η_ℓ will give all the ℓ^{th} partial cross-sections (total, reaction, and elastic scattering).

$$\frac{\sigma t}{\pi R^2} = \frac{2\ell+1}{x^2}\, 2 R_\ell\,(1 - \eta_\ell)$$

$$\frac{\sigma c}{\pi R^2} = \frac{2\ell+1}{x^2}\,(1 - |\eta_\ell|^2)$$

$$\frac{\sigma s\ell}{R^2} = \frac{2\ell+1}{x^2}\,|1 - \eta_\ell|^2$$

A program has been written which finds the value of the wave function $\mu_\ell = v_\ell + iw_\ell$ by means of a power series for w and v. Another program is being worked on which will generate the wave function from these starting values by using the Milne Predictor-Corrector formula. At the same time the function is generated the integrals in the expression for $\cot\delta_\ell$ will be computed. As soon as this program has been tested it will be combined with the first one in such a way that given any x, X_o, S and δ the cross sections will be found for ℓ from 0 to 6.

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

247 C. SURFACE PRESSURE PREDICTION

In the past a considerable amount of work has been done by Prof. Wadsworth's D.I.C. Statistical Laboratory at M.I.T. in the prediction of surface pressure by means of linear functions of present and past values of pressure, taken over a network of points on the map. As a collateral study by Prof. Wadsworth's group, it was found that a large sector of the pressure map could be represented adequately as a geometrical surface, expressable analytically as a general polynomial in the coordinates of the points, regarded as lying on a plane surface. By this device, it was possible to reduce a network of 91 observation points to a set of 15 orthogonal functions, namely, the coefficients of the polynomial expression. Using these orthogonal functions in place of direct pressure observations, Prof. Malone carried Wadsworth's method of pressure prediction a step further, with very encouraging results (cf. problem 155).

An entirely independent approach to this problem has been made by the so-called numerical forecasting group. The technique employed by this group involves the numerical solution of differential equations with stated boundary conditions. The type of solution depends upon the physical assumptions made in setting up the differential equations, but in general the form of solution is largely linear in the pressure values. However it does contain certain quadratic terms. The results of Prof. Malone proved to be at least as good as those obtained by the numerical forecasting group, but it seemed desirable to exploit the idea of quadratic functions further.

The object of the present study by the D.I.C. Statistical Laboratory is to evaluate the introduction of the quadratic component into the general linear scheme of Wadsworth and Malone. The pressure surface is represented by a set of orthogonal functions, and then the squares and products of the most important of these functions are incorporated as representative of the general quadratic contributions.

249 C. FLIGHT INTERCEPTOR CONTROL

This problem is concerned with a systems-analysis investigation of the dynamics and control of an interceptor. The system is described by thirteen differential equations, which were solved on Whirlwind I by the Gill method. The Whirlwind I solution has been completed, and its digital results served as a standard check for later analogue computations done on the M.I.T. Flight Simulator of the Dynamic Analysis and Control Laboratory.

250 C. TRANSLATION PROGRAM FOR THE NUMERICALLY-CONTROLLED MILLING MACHINE

The M.I.T. Numerically-Controlled Milling Machine (NCMM) is a standard milling machine modified so that it can be automatically controlled by numerical instructions punched in a paper tape. A complicated sequence of motions of the cutting tool may be entirely specified in speed and direction on the punched tape, and no manual intervention by a human operator is required during the cutting.

The data punched in the control tape must appear in numerical form. This requires, in general, that the precise x, y, and z coordinates of all significant points on the work be computed. The tape instructions specify the motion of the center of the cutting tool, while cutting occurs at the periphery of the cutter and not at its center. This necessitates a further transformation of the points on the work to account for the offset of the cutter center. These calculations, even for a relatively simple cutting job, are tedious and time-consuming. The task of preparing a control tape is even further complicated by the fact that the tapes must be punched in an octal code in which the final instructions take a form quite different from the numbers used during their calculation.

In order to reduce the time required for the preparation of NCMM tapes and to minimize tape errors, a procedure for utilizing a digital computer has been found feasible. A translation program is being written for Whirlwind I which accepts a description of the work in symbolic form and which produces automatically the required NCMM control tape. The calculations and transformations which were described in the preceding paragraph are executed automatically by the Whirlwind I computer.

The first form of the translation program has, for simplicity, been limited to curves consisting solely of straight lines and circles in two dimensions. Straight-line motion in the third dimension has been included, in a somewhat restricted form.

A brief description of the vocabulary accepted by this program follows. All symbols are typed on the M.I.T. Flexowriter exactly as they appear in the description.

Tags

Points, straight lines, and circles will be tagged using a tag assignment of one of the forms given in the table below. A tag* may not appear after the = symbol unless it has already been assigned.

- - - - - - - -

*A tag consists of the letter p(point), c(circle), or s(straight line), followed by any integer i such that $0 \leq i \leq 255$. The integers serve only to distinguish one tag from another, and have no numerical significance.

By convention, the positive direction on a straight line is specified by the order of the two points used in tagging it, and is the direction from the first point to the second point. The positive direction on a circle is always counter clockwise. Starting from the point of minimum x and proceeding along a curve in its positive direction, the first intersection with a second curve is the near (N) intersection; the other is the far (F) intersection. Two circles, or a line and a circle are said to be tangent (T) when they have one and only one intersection and their positive directions coincide at the point of intersection; they are antitangent (A) if their positive directions do no coincide at their only point of intersection.

Points

<table>
<tr><th>Typed Symbols</th><th>Meaning</th></tr>
<tr><td>p16 = -2.734, 6.2545</td><td>coordinates</td></tr>
<tr><td>p35 = s12 | s17</td><td>intersection of two lines</td></tr>
<tr><td>p12 = N s1 | c12
p12 = F s1 | c15</td><td>intersection of a line with a circle</td></tr>
<tr><td>p15 = N c3 | c5
p15 = F c3 | c16</td><td>intersection of two circles</td></tr>
<tr><td>p19 = c17 | 82°</td><td>on circle, angle with positive x axis</td></tr>
</table>

Lines

<table>
<tr><th>Typed Symbols</th><th>Meaning</th></tr>
<tr><td>s3 = p1 | p2</td><td>two points</td></tr>
<tr><td>s2 = p1 | Tc2*
s2 = p1 | Ac3</td><td>through point, tangent to circle</td></tr>
<tr><td>s1 = Ac1 | Ac3
s2 = Tc1 | Ac3
s3 = Ac1 | Tc3
s4 = Tc1 | Tc3</td><td>tangent to two circles</td></tr>
<tr><td>s3 = p12 | 73°</td><td>point, angle with positive x axis</td></tr>
</table>

Circles

<table>
<tr><th>Typed Symbols</th><th>Meaning</th></tr>
<tr><td>c7 = p1, 2.7405</td><td>center, radius</td></tr>
<tr><td>c2 = p1 | Tc1
c2 = p1 | Ac3</td><td>center, tangent to another circle</td></tr>
<tr><td>c5 = p5 | s2</td><td>center, tangent to line</td></tr>
</table>

Cutting Instructions

After the significant points, lines, and circles on the work have been tagged, the actual cuts required will be specified in terms of them. The cutting instructions take the following form:

- - - - - - - -

*These tag assignments may be typed as s2 = Tc2 | p1 and s2 = Ac3 | p1 in order to reverse the positive direction on the line.

Symbols Typed	Meaning
7.5, p3, -6.214	move at 7.5 in/min feedrate in a straight line to p3, at the same time lowering the cutter 6.214 in.
15, +c1, p2, 0.3	move at 15 in/min along circle c1 in its positive direction, to p2, at the same time raising the cutter 0.3 in.
7.5, -c3, p5	move at 7.5 in/min along circle c3 in its negative direction to p5 without vertical motion of the cutter
STOP	stop the NCMM (punch feedout)
END	signifies end of Flexowriter instruction tape

The initial cutting instruction assumes the tool is at x = 0, y = 0. Subsequent cutting instructions assume the tool to be where the preceding instruction left it.

Special Words

Special words, used to provide information needed in calculating the NCMM instructions, must appear on the input tape as follows:

RIGHT	Tool to right of cut
LEFT	Tool to left of cut
TOOL RADIUS = 0.5	
TOLERANCE = 0.0005	

The translation program is, at present, about 75% complete. It is expected that the routine will be completely tested and available to NCMM users by July, 1955. This study is being carried out by A. Siegel of the Digital Computer Laboratory staff.

251 B. DYNAMICS AND CONTROL OF PACKED DISTILLATION COLUMNS

A large amount of data has been taken on a packed distillation column in order to determine which, out of a fairly large number of physical parameters, are those which can best be used to describe and predict the dynamics of packed columns affecting the composition of the tower output.

In order to test out a set of difference equations which have been developed, Whirlwind I is being programmed to simulate the actual packed column.

One portion of the theoretical equations, concerned with the distributed mixing of liquids, has already been tested out on the computer and checked against measured data. This has taken about two hours of computer time.

The difference equations are concerned with the following physical effects:

1) mass transfer;
2) heat transfer;
3) fluid and vapor flow.

All of these effects occur simultaneously in every section of the column. The numerical model involves the breaking down of the column into N physical sections and picking the increments of both time and distance small enough so that the effects can be considered independently within each section.

The complete program has not yet been completed, and therefore no conclusive results can be stated at this time. The study is being carried out by H. M. Teager of the Electrical Engineering Department.

252 N. ANALYSIS OF TWO STORY STEEL FRAME BUILDING

A report on this problem is given in section 2.2 of Part I.

256 C. WWI-ERA 1103 TRANSLATION PROGRAM

A two pass input translation program has been written by members of the Digital Computer Laboratory at M.I.T. to simplify the machine coding problem for programmers working on Problem 126. It will allow them to code programs for the Univac Scientific Model 1103 in a mnemonic (two letter) operation code and to use either or both symbolic and integer addresses. The translation program accepts Flexo-coded punched paper tape as input and produces a seventh-level bi-octal punched paper tape acceptable as input to the 1103 computer. The program operates on the Whirlwind I computer at M.I.T. and was written under the sponsorship of the Digital Computer Laboratory and Project DIC 7138 of the Servomechanisms Laboratory at M.I.T. It will be used in the coding of the large data reduction program which is being developed at the Servomechanisms Laboratory under Problem 126 and which is expected to be run on the Eglin Field 1103.

The 1103 computer is a large two address computer containing 1024 or 4096 registers of random access memory and 16384 registers of directly addressable drum memory. Each register consists of 36 binary digits of which, in most instructions, 6 bits are used to designate the operation and two sets of 15 bits designate the two addresses. In some cases the two addresses can be divided so that as many as four "addresses" can occur in the instruction. The registers in the arithmetic element of the computer are directly addressable. Both 7-hole punched paper tape and punched cards can be used for input and output.

The following is a brief summary of the vocabulary and syntax of the translation program:

A. Characters

The words in the vocabulary of the translation program will be composed of suitably punctuated and terminated syllables of letters and digits punched in standard Flexowriter code on paper tape.

B. Words

Three classes of words are defined. The first class consists of all those words which occupy storage registers in the translated program. These words are instructions, with zero to four addresses, or (integer) numbers. We call this class of words polysyllabic storage words.

The second class, called polysyllabic control words, consists of current address assignments, symbolic address assignments, and starting address assignments. These words influence the form, location, and operation of the translated program but do not themselves occupy registers of storage.

The third class of words, called special words, are used for miscellaneous control and identifying purposes. They are the title, the number base indicator, and the comment word.

The words of the first two classes are combinations of these syllables: operations, symbolic address tags, integers and the literal addresses "q," "a," and "b." These words are distinguished solely by the internal and terminal punctuation. These characters are "+", "-", "=", ",", ".", " | ", the tab, and the carriage return.

C. Syllables

1. Operations. These are the mnemonic lower case two-letter pairs corresponding to the standard listing of the 1103 operation code.

2. Symbolic address tags. These are three character digit and letter combinations.

3. Literal addresses. The letters "q", "a", and "b" refer to the quotient, right accumulator and left accumulator, respectively.

4. Integers. Integers may have any value up to 2^{35}-1, so long as the completely evaluated word, or part of a word, of which the integer is a syllable, fits into the number of bits meaningfully available in the translated word.

D. Polysyllabic Storage Words

1. Instructions. An instruction word always has the operation code as the initial syllable. Zero to four addresses may follow; the translation program will decide where to position the addresses, bit-wise, in the word if a meaningful number of addresses is given. The addresses are separated by commas and the last is terminated by a tab or carriage return. Each address is written as the sum of symbolic address tags, literal addresses, and integers, where the manner of summation is indicated by prefixing each syllable of the address by a plus or minus sign.

2. Numbers. A number has the form of an address of an instruction word and is terminated by a tab or carriage return. The value of the translated number must be less than 2^{35}-1.

E. Polysyllabic Control Words

1. Current address assignments. A current address assignment has the form of an address of an instruction word except that here the terminating character is a vertical bar: " | ". This word causes the next polysyllabic storage word to occupy the register of 1103 storage, high-speed or drum, whose address is the value specified in the current address assignment. Successive storage words will thereafter go into successive registers of storage until another current address assignment occurs.

2. Symbolic address assignments. This word consists of a single symbolic address tag and is terminated by a comma: ",". The value assigned to the tag is the location which a polysyllabic storage word would occupy if one were the next word on the Flexo tape; this is true whether or not one occurs there. A tag can be reassigned several times in a program, the last value being used in the translated program. All reassigned tags are indicated as such by the translation program.

3. Starting address assignment. A starting address assignment word must occur at the end of each Flexowriter program tape. It has the form of a single address instruction word, where the place of the operation code is taken by the syllable: "start at." The value of the starting address indicates where operation of the translated program is to begin.

F. Special Words

1. Titles. A title is used for identifying Flexo tapes and logging the translation of the tapes on Whirlwind I. A title must occur at the beginning of each tape.

2. Number base indicator. This word is written as "base k," where k is any integer from one to ten. All following integer syllables in the program will be converted to binary from this base, until another base indicator occurs. A "base 10" is assumed initially.

3. Comment word. This word is totally ignored by the translation program and is provided so that comments may appear on a program print when a program tape is printed. This word must have a vertical bar occurring initially and is terminated by a tab or carriage return. Any Flexo character may occur in between.

G. Symbolic Addresses

If a programmer decides that he needs to modify a section of his program and does not desire to reproduce the entire Flexo tape in order to make the required deletion and insertion, then he need only append a tape of the modified section to the main tape and have both translated together. The translation program will then effectively insert the appended section of the program into the program, expanding or contracting the original section of the program to occupy the same number of storage locations as the replacement. The facility is thus available to insert or delete words in a program by making modifications at the end of the tape.

At the end of each program translation all the values for all the symbolic addresses assigned in the program are listed. All unassigned and incorrectly assigned symbolic addresses are also listed. Hence a

programmer has a complete record of the storage locations used by his program, as well as of the effect of modifications on the program.

H. Error Detection

Illegal combinations of characters are detected, and so recorded, by the translation program wherever possible. The locations of the errors are given in terms of the most recent symbolic address or current address assignment.

I. Present Status

The basic elements of the translation program are now working. Translated program tapes are complete except for visual titles, but the programs for printing the symbolic address tables and the detected programmer's mistakes have not yet been tested. The WWI utility input program must also be modified in order to allow the translation program to operate in the same automatic manner as CS and the other WWI systems. All of this work will be completed in the next quarter.

258 C. DYNAMIC ANALYSIS OF AN AIRCRAFT INTERCEPTOR

This problem involves systems analysis of an aircraft interceptor control system and is being conducted to determine the adequacy of certain force and moment equations to describe the motion of an aircraft. The system is described by eight differential equations to be solved by the Gill method. Four solutions using different types of inputs to the control will be made by Whirlwind I. These solutions also will serve as a standard for analogue computations to be performed on the M.I.T. Flight Simulator of the Dynamic Analysis and Control Laboratory.

The general program for the first Whirlwind solution has been written and tested and is now ready to be run. The second and third solutions will use the same basic program with minor changes necessitated by the changes of input. The fourth solution is being programmed separately and is now ready for testing.

260 N. ENERGY LEVELS OF DIATOMIC HYDRIDES

A study of the electronic energy of the OH molecule including configuration interaction is under way. The energy will be calculated as a function of internuclear distance. The ground state of the molecule is $^2\pi$.

The basic set of one-electron orbitals are the hydrogen 1s ground state function and the 1s, 2s, and sp Hartree Fock[1] wave functions of oxygen. The notation followed is to call oxygen 1s = s, oxygen 2s = σ, oxygen 2p = p, and hydrogen 1s = h.

Use is being made of the Whirlwind I digital computer to calculate one- and two-electron integrals of the form:

$$(i\,|f_1|\,j) = \int \varphi^*_i(1)\, f_1\, \varphi_j(1)\, d\tau_1$$

$$(ij\,|g_{12}|\,k) = \int \varphi^*_i(1)\, \varphi^*_j(2)\; g_{12}\, \varphi_k(1)\, \varphi_\ell(2)\, d\tau_1\, d\tau_2$$

$$(ij\,|g_{12}|\,k) = \int \varphi^*_i(1)\, \varphi^*_j(2)\; g_{12}\, \varphi_\ell(1)\, \varphi_k(2)\, d\tau_1\, d\tau_2$$

where the φ_i's are the one-electron wave functions and f_1 and g_{12} the one-and two-electron operators respectively. These integrals are easily calculated by using the program written by F. J. Corbató.[2] The most difficult of the integrals takes about 5 seconds of machine time while the others take considerably less.

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1. D. R. Hartree, W. Hartree and B. Swirles, Trans. Roy. Soc. (London) A238,229 (1939).

2. F. J. Corbato, Quarterly Progress Report, Solid State and Molecular Theory Group, M.I.T., April 15, 1955.

So far several hundred of these integrals have been computed by Whirlwind. Many more will be done before the task is done. This work is being carried out by A. J. Freeman of the Solid State and Molecular Theory Group.

262 N. EVALUATION OF TWO-CENTER MOLECULAR INTEGRALS

The problem to be solved by Whirlwind is the numerical evaluation of different types of two-center integrals between 15 and 25, 2p atomic orbitals for the values of internuclear distance R. This study is being carried out for the hydrogen molecule.

The first step, which is the evaluation of one-electron integrals, has been completed. Routines developed for one-electron integral evaluation by F. J. Corbató of the M.I.T. Physics Department were used.

The results of this problem will be included in the Ph.D. thesis of H. A. Aghajanian of the M.I.T. Solid State and Molecular Theory Group.

263 C. FLIGHT PATH OF AN AIRCRAFT DURING PULL-UP

This problem is concerned with the solutions of a set of five differential equations which describe in terms of velocity, altitude and angles, the flight path of an aircraft during pull-up. In addition, thirteen quantities are to be calculated from each solution of the differential equations.

At first, it was thought that the problem was to be solved for one set of initial conditions. Consequently, the program used was the "George I" interpretive program devised under Problem 108 by J. H. Laning and N. Zierler of the Instrumentation Laboratory. This program translates mathematical equations into Whirlwind code and requires no programming by the programmer, except a knowledge of certain logical procedures.

When it was decided to solve the problem for thirty sets of initial conditions, it became apparent that the computing time using "George I" would be prohibitive. Therefore, a CS interpretive program in (24,6) arithmetic was written by Charles Block of the Instrumentation Laboratory. With the aid of a small amount of hand computation and the IBM Card Program Calculator at the Instrumentation Laboratory, the computational sections of the CS program have been cleared of all programming errors. What remains to be done before the complete run of the solutions for the thirty sets of intial conditions can be made is to remove some programming errors in a cycling routine.

285 B,N. APPLICATION OF AUGMENTED PLANE WAVE METHOD TO CHROMIUM CRYSTAL

Modifications are being made in Dr. D. Howarth's routine (described in Summary Report No. 37 under Problem 147) which obtains the curves of energy versus plane wave energy so that integrated wave functions for any energy and angular momentum appear on the scope. A routine has been written which calculates and prints potentials and $2Z_p$ for potentials written as a linear combination of exponentials multiplied by powers of the radius. The routine has been applied to the potential for chromium crystal supplied to Mr. M. M. Saffren of the Solid State and Molecular Theory Group by Dr. Robert Parmenter of R.C.A.

1. PUBLICATIONS

Project Whirlwind technical reports and memorandums 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-41	An ERA 1103-WWI Translation Program	1-4-55	J. M. Frankovich
DCL-47	Payroll Demonstration Routine	1-13-55	B. Riskin
DCL-48	Automatic Scope Output Requests	1-25-55	A. Siegel and S. Best
DCL-49-1	A Proposed Translation Program for the Numerically Controlled Milling Machine	1-26-55	A. Siegel
DCL-57	Calendar Demonstration Routine	2-28-55	R. J. Hamlin and E. Raiffa
DCL-58	Program for Solving Secular Equations	3-15-55	F. J. Corbató
DCL-61	Report on the WWI-ERA 1103 Input Translation Program (Published in the ERA 1103 Newsletter)	3-15-55	J. M. Frankovich
DCL-62	Report 18 January Meeting at MIT of WWI-1103	3-15-55	J. M. Frankovich
DCL-63	Annotated Prints of CS Flexo Program Tapes	3-10-55	J. M. Frankovich

2. 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 13 groups visited the computer installation. Included in these groups were:

January 6	Professor Hansen's Class, Civil Engineering Department, M.I.T.
January 14	Professor P. J. Rulon's Class, Mathematics Dept., Harvard
January 21	Reynolds Metal Company
February 4	Atlantic Gelatin Company
February 14	Union Carbide and Carbon Company
February 23	American and New York Tel and Tel
March 22	Air Force Reserve Research and Development Group

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 65 persons visited the Laboratory at the Open House demonstrations. These persons represented members and friends of the M.I.T. community, the Retina Foundation, the University of Illinois and Harvard University.

During the past quarter there were also 15 individuals who made tours of the computer installation at different times. These individuals represented French Morocco Realis Elect., Raytheon Mfg Co., Electronics Corp., A. O. Smith Corp., Dupont, Rensselaer Polytechnic Institute, University of California at Los Angeles, Harvard, Yale, and M.I.T.

PERSONNEL OF THE PROJECTS

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Sidney D. Drell	Physics
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Research Associate:

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Research Assistants:

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Andrew T. Ling	Mechanical Engineering
M. Douglas McIlroy	Mathematics
John F. O'Donnell	Chemical Engineering
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Anthony Ralston	Mathematics
Manuel Rotenberg	Physics
Leo Sartori	Physics
Aaron Temkin	Physics
Marius Troost	Chemical Engineering
Arnold Tubis	Physics
Jack L. Uretsky	Physics
Keeva Vozoff	Geology and Geophysics

PROJECT WHIRLWIND

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