

MACHINE METHODS OF COMPUTATION
and
NUMERICAL ANALYSIS
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and

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FOREWORD

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

Project on Machine Methods of Computation and Numerical Analysis

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

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

Project Whirlwind

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

The Whirlwind I Computer

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

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

PART I

Machine Methods of Computation and Numerical Analysis

1. GENERAL COMMENTS

The summer quarter marks a turning point in the activities of the Project. In place of the personnel who reported their final results at the end of the last quarter, new personnel are being introduced to the computing facilities of the Institute. As always, these new members have special interests in various sciences and common interest in the techniques of modern computing machinery.

Most of the reports in the following pages represent projects that continued in progress over the summer in the fields of mathematics and physics. One new and one final report on projects initiated in the engineering and mathematics departments are also included. The common objective of each of these is to extend the techniques of numerical analysis and computing into some field of application. In achieving this objective, the techniques themselves are enriched with useful sub-routines which then become available to other workers.

2. GRADUATE SCHOOL RESEARCH

2.1 Index to Reports

Title	Page
Eigenvalues in a Spheroidal Square Well	7
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Energy Bands in Graphite	9
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2.2 Progress Reports

EIGENVALUES IN A SPHEROIDAL SQUARE WELL

It will be recalled [1] that this problem is concerned with the solution of the matrix equations

$$\sum_{\nu} A_{\mu\nu}(h) a_{\nu} = 0$$

where the $A_{\mu\nu}$ depend upon the energy parameter h through combinations of spheroidal wave functions. The eigenvalues h_k are determined by the usual condition that the infinite determinant

$$\det A_{\mu\nu}(h) = 0.$$

The procedure that was followed was to find the "eigenvalues" of a set of $n \times n$ determinants of increasing size in the hope that the successive approximations $h_k^{(n)}$ would converge rapidly as a function of n .

The result was unexpected. It was found that for the well distortions of interest ($\epsilon \sim .7$ where $\epsilon = \text{interfocal distance/major axis}$) the values of $h_{kl}^{(n)}$ did not change by more than a per cent or two for $1 \leq n \leq 4$. Here $h_{kl}^{(1)}$ is the l 'th zero of the diagonal element A_{kk} .

Since it took better than fifteen minutes for Whirlwind to find a typical $h_{kl}^{(4)}$ as contrasted with 4-5 minutes for the corresponding first-order approximation, I decided to be content with the lesser accuracy in the hundred or so eigenvalues which were required.

Computations are about 80 per cent complete for a nucleus of $A = 160$, well-depth 40 mev, and nuclear radius $1.5 A^{1/3} \times 10^{-13}$ cm. Five different eccentricities are being used, ranging from $\epsilon = .5$ oblate to $\epsilon = .8$ prolate. The energies thus obtained will be used to compute the variation

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in the total energy as a function of the distortion.

Jack L. Uretsky

Reference:

- [1] Machine Methods of Computation and Numerical Analysis, Quarterly Progress Report No. 15, March 15 (1955) p. 19. Also Report No. 16, June 15 (1955) p. 21.

ATOMIC WAVE FUNCTIONS AND ENERGIES

The program outlined in Quarterly Progress Report No. 16 has been abandoned and the computation of energies has been completed using a lengthier but more straightforward and accurate procedure.

The method mentioned in the preceding Progress Report gives six significant figures for the first term of non-isoelectronic sequence but loses accuracy rapidly for the higher terms. The method used in its place consists simply of first holding "b" and "c" constant and finding the best value of "a" to within ± 0.02 and then doing similarly for "b" and "c" with $\Delta "b" = \pm 0.02$ and $\Delta "c" = \pm 0.003$. This process is then iterated as many times as is necessary to give six significant figures. The process for one atom takes about one minute of machine time. The computation of the energy is divided up into an "a" dependent part, a "b" dependent part, etc. so that we need not go through the full energy evaluation procedure each time as we go along one of the parameter axes.

Listed below are some results which are compared to previous computation done on I.B.M. W = energy in atomic units.

	I.B.M. Results			
	a	b	c	W
C _I	3.51	3.18	0.965	75.256
N _{II}	3.24	2.892	1.027	107.655
O _{III}	3.01	2.55	1.003	146.080

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	Whirlwind Results			
	a	b	c	W
C _I	3.44	3.10	0.942	75.257
N _{II}	3.20	2.81	1.007	107.657
O _{III}	3.00	2.53	1.023	146.081

The programming of the variational procedure has taught the writer of this report one major lesson--namely, that it is usually best to use the most straightforward procedure possible instead of more elaborate ones whose value is evident only in special cases. A glance at the previous progress reports on this problem will bear the above statement out.

Arnold Tubis

ENERGY BANDS IN GRAPHITE

The tight-binding calculation of a two-dimensional graphite model is being continued. As was described in a previous report [1], three-center integrals were found to be necessary and these are being evaluated. These integrals are being done by the method of expanding the orbitals around another center and expressing the result as a series of Gegenbauer polynomials with numerical integrals as coefficients. For several cases the series were found after ten terms to be only moderately convergent. By empirically observing that the coefficients in a given series are roughly in a geometric progression, it is possible to greatly enhance the convergence by approximately summing the infinite tail of the series using expressions derived from the generating function of the Gegenbauer polynomials. To avoid numerical errors, a computer program has been written to accomplish this latter process and is currently being tested.

Fernando J. Corbato

GRADUATE SCHOOL RESEARCH

Reference:

- [1] F. J. Corbato, Quarterly Progress Report, Solid-State and Molecular Theory Group, M.I.T., July 15, 1955, p. 8.

COULOMB WAVE FUNCTIONS

The methods of getting the regular and irregular Coulomb wave functions outlined by Abramowitz (Phys. Rev. 98, 1955) requires a knowledge of the irregular function g_L for $L = 0$. Up to now the problem has been one of computing the irregular function

$$g_0 = \frac{1 - e^{-2\pi\eta}}{2\pi\eta} \int_0^1 \left\{ \rho^{2\eta} \tan^{-1} \left(\frac{\log \frac{1+t}{1-t}}{\rho} \right) - \rho \sin \left[\rho t - \eta \log \frac{1+t}{1-t} \right] \right\} dt$$

with sufficient accuracy to be useful in any iterative or interpolative procedure for finding other Coulomb wave functions. To this end new subroutines were written for all the functions which occur in the above integrand. These routines are accurate to 8 and 9 places for almost all relevant values of the argument. One additional difficulty is the fact that the second term in the integrand is not well behaved as $t \rightarrow 1$. It oscillates more and more rapidly in this limit, and the question arises, how to get a good estimate of its contribution to the whole integral. Dr. Abramowitz, when he was at M.I.T. during the summer for a week, suggested the following device, which we think largely eliminates this difficulty. From the second term of the integral (taken along the transition line $\rho = 2\eta$ for convenience, and this can be done for any value of ρ and η) subtract and add the limiting form of the integrand.

i.e. $\lim_{t \rightarrow 1} \left[t - \frac{1}{2} \log \frac{1+t}{1-t} \right] = 1 - \frac{1}{2} \log \frac{2}{1-t}$ Thus

$$\int_0^1 \sin \left\{ 2\eta \left[t - \frac{1}{2} \log \frac{1+t}{1-t} \right] \right\} dt = \int_0^1 \left\{ \sin \left(2\eta \left[t - \frac{1}{2} \log \frac{1+t}{1-t} \right] \right) - \sin \left(2\eta \left[1 + \frac{1}{2} \log \frac{1-t}{2} \right] \right) \right\} dt + \int_0^1 \sin \left(2\eta \left[1 + \frac{1}{2} \log \frac{1-t}{2} \right] \right) dt$$

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The second integral can be done analytically:

$$\int_0^1 \sin \left(2\eta \left[1 + \frac{1}{2} \log \frac{1+t}{2} \right] \right) dt = \frac{\sin 2\eta}{1 + \eta^2} \left[\cos (\eta \log 2) - \eta \sin (\eta \log 2) \right] - \frac{\cos 2\eta}{1 + \eta^2} \left[\sin (\eta \log 2) + \eta \cos (\eta \log 2) \right]$$

The trick is to evaluate the integral in the above expression numerically, for it now has the property that its oscillations rapidly vanish near the end point $t = 1$, for the two sines in the integrand approach each other. Thus, although the above integral has a somewhat more complicated analytic form, it is much better behaved than the original integral and one should be able to get a much better numerical estimate of it. The integrated terms can be done once and for all.

The numerical technique we have in mind is a Gaussian quadrature. But it must be kept in mind that all these methods are severely handicapped on Whirlwind where the maximum one can store is ten decimal digits.

Zoltan Fried
Aaron Temkin
Arnold Tubis

CRACK GROWTH IN A DUCTILE MATERIAL

The stress pattern within a bar with an axial crack under torsional loading must be found as an initial step in investigating the processes by which cracks grow in a ductile material. Due to the complexity of the problem because of the deviation from linearity in the plastic region, the use of a high-speed computing method is necessary. The problem is being studied in order that it may be presented in a form adaptable to the Whirlwind machine.

Joseph B. Walsh

THEORY OF STOCHASTIC PROCESSES

The purpose of this report is to present a theorem which has arisen in the theory of enchainned stochastic processes. Some ideas relating to this theorem have been presented previously in these reports [1] and have found application in the theory of cosmic ray showers [2,3].

Let $(\Omega, \mathcal{B}_\Omega, P)$ be a probability space and let $(\Gamma, \mathcal{B}_\Gamma)$, $(\gamma, \mathcal{B}_\gamma)$ be measurable spaces. The symbols Ω, Γ, γ represent some general spaces made up of points ω, G, g , respectively. For each real $x \geq 0$, let $\mathcal{G}(x), \mathcal{F}(x)$ be measurable functions defined Ω to Γ, γ , respectively. The collections $\mathcal{G} \equiv \{\mathcal{G}(x), 0 \leq x < \infty\}$, $\mathcal{F} \equiv \{\mathcal{F}(x), 0 \leq x < \infty\}$ will be called stochastic processes.

In order to state the theorem of interest in this paper, it will be necessary to make the following assumptions:

- (1) \mathcal{G} is a Markovian process.
- (2) The σ -field of ω events induced by $\mathcal{F}(x)$ is contained in that induced by $\mathcal{G}(x)$ for all $x \geq 0$.
- (3) For all $x, y, x \geq 0, y \geq 0, \mathcal{F}(x) = \mathcal{F}(y)$ if and only if $\mathcal{G}(x) = \mathcal{G}(y)$.
- (4) For all $x, y, x \geq y \geq 0, \mathcal{G}(x) = \mathcal{G}(y)$ if and only if for all $z, x \geq z \geq y \geq 0, \mathcal{G}(x) = \mathcal{G}(z)$.
- (5) The space γ to which $\mathcal{F}(x)$ is defined is denumerable and $g \in \mathcal{B}_\gamma$ for all $g \in \gamma$.
- (6) Corresponding to the process \mathcal{G} there exists for all $x, y, x > y \geq 0$, a transition function, $P_1(B_\Gamma, x | G, y)$, such that (1) as a set function of $B_\Gamma \in \mathcal{B}_\Gamma$ it is non-negative and completely additive, (2) as a point function of $G \in \Gamma$ it is measurable with respect to \mathcal{B}_Γ and (3) for each set $B_\Gamma \in \mathcal{B}_\Gamma$ and each $x, y, x > y \geq 0, P_1(B_\Gamma, x | \mathcal{G}(y), y)$ is the conditional probability of the event $\mathcal{G}(x) \in B_\Gamma$ given $\mathcal{G}(y)$ with probability 1.
- (7) $P_1(B_\Gamma, x | G_0, 0)$ satisfies the linear, temporally homogeneous diffusion equation,

$$\frac{\partial}{\partial x} P_1(B_\Gamma, x | G_0, 0) = \int_\Gamma P_1(dG, x | G_0, 0) \pi(G \rightarrow B_\Gamma) - \int_{B_\Gamma} P_1(dG, x | G_0, 0) \alpha(G),$$

$B_\Gamma \in \mathcal{B}_\Gamma, G_0 \in \Gamma, 0 < x < \infty$, where

$$\pi(G \rightarrow B_\Gamma) = \lim_{(x-y) \rightarrow 0} P_1(B_\Gamma, x | G, y) / (x-y), \quad G \notin B_\Gamma$$

$$\pi(G \rightarrow G) = 0, \quad \alpha(G) = \pi(G \rightarrow \Gamma).$$

From these assumptions it follows that there is a transition function, $P_2(g, x | g', y)$, corresponding to the process \mathcal{F} , which plays the analytical counterpart of the conditional probability of the event $\mathcal{F}(x) = g$ given $\mathcal{F}(y)$. The purpose of the theorem of this report is to establish that a certain condition on the function $\alpha(G)$ is sufficient for insuring that $P_2(g, x | g_0, 0)$ has a specified analytical form.

It is necessary to define a special stochastic process. This process is simply a tool for computing the chance that if \mathcal{F} arrived at the state g for some $x > 0$, then it did so by passing through a certain specified sequence of points of the denumerable space γ . Let $\pi(g)$ represent the space of all finite sequences of distinct points in γ ending with g . That is, if $p \in \pi(g)$, there is some finite sequence $g_0, g_1, \dots, g_{N-1}, g$ (where N may be different for different p) such that $p \equiv (g_0, g_1, \dots, g_{N-1}, g)$. For each $g \in \gamma$, define a random variable $\mathcal{P}(g)$ such that $\mathcal{P}(g) = p = (g_0, g_1, \dots, g_{N-1}, g)$ if and only if (1) for some set (x_1, x_2, \dots, x_N) , $x_k > x_{k-1} > 0, \mathcal{F}(0) = g_0, \mathcal{F}(x_1) = g_1, \dots, \mathcal{F}(x_{N-1}) = g_{N-1}, \mathcal{F}(x_N) = g$ and (2) for all $x, x_N \geq x \geq 0, \mathcal{F}(x) = g_k$ for some $k = 0, 1, \dots, N, g_N = g$. In words, $\mathcal{P}(g) = p$ when the sequence of points which \mathcal{F} has passed through in getting to g is p . To complete the definition it is necessary to impose the normalizing condition

$$\sum_{p \in \pi(g)} P[\mathcal{P}(g) = p] = 1.$$

Now define the process with the statement

$$\mathcal{P}_F(x) \equiv (\mathcal{P}[F(x)], F(x)), \quad x \geq 0.$$

$\mathcal{P}_F(x)$ is thus a random variable defined to the space of all pairs $(p, g), p \in \pi(g), g \in \gamma$. $\mathcal{P}_F(x) = (p, g)$ is the event that at x $F(x) = g$ and the process F arrived at g by passing through the sequence p . It is clear that for all $g \in \gamma$

$$P(F(x) = g) = \sum_{p \in \pi(g)} P(\mathcal{P}_F(x) = (p, g)).$$

The theorem can now be stated. In the statement of the theorem " $*$ " represents the operation of convolution.

Theorem: Suppose assumptions (1)-(7) hold. If for each $g \in \gamma$ $\alpha(g) = \text{const.} = \alpha(g)$ for all $G \in g$, then \mathcal{P}_F is Markovian and

$$P_2(g, x | g_0, 0) = \sum_{p \in \pi(g)} \left[\prod_{k=1}^N \frac{\bar{m}(g_{k-1} \rightarrow g_k)}{\alpha(g_{k-1})} \right] \alpha(g_0) e^{-x\alpha(g_0)} * \dots * \alpha(g_N) e^{-x\alpha(g_N)},$$

$g_N = g$, where for each fixed $g' \in \gamma$, $\bar{m}(g' \rightarrow g) / \alpha(g')$ is a probability measure over the space γ .

The proof of this theorem will be contained in a paper yet to be published entitled, "The Concept of Enchainment--A Relation Between Stochastic Processes."

Bayard Rankin

References:

- [1] Machine Methods of Computation and Numerical Analysis, Quarterly Progress Report No. 14, December 15 (1954), p. 45.
- [2] *ibid.* Report No. 13, September 15 (1954), p. 48.
- [3] *ibid.* Report No. 14, December 15 (1954), p. 11.

2.3 Final Reports

CALCULATION OF NUMBERS OF STRUCTURES OF RELATIONS ON FINITE SETS

A table of numbers of structures of dyadic relations has been calculated on Whirlwind I. The problem was taken up

primarily to test a multi-register arithmetic program for manipulating numbers of arbitrary length. Thus, we obtained exact integer answers to this problem, even though these results are as high as 10^{60} . The results are given here completely written out, although they have primarily curiosity value.

The problem, as described in a previous report, [2], concerns dyadic relationships holding among a set of n objects. A complete relationship is specified by an $n \times n$ 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 admissible arrays of 1's and 0's in the incidence matrix. With no further restrictions, we see that the answer is 2^{n^2} , but in this figure we have included many "orbits" of isomorphic structures which can be permuted into one another by renumbering the objects of the set. The task at hand is to find how many orbits of non-isomorphic structures exist. Davis [1] has shown that this number is

$$(1) \quad \text{str}_n = \frac{1}{n!} \sum_{\tilde{\pi}} b(\pi) 2^{d(\pi)}$$

where the summand is to be evaluated for one permutation, $\tilde{\pi}$, from each conjugate class of the symmetric group of permutations on n objects. Every member of a conjugate class has the same distinct disjoint cycle scheme specified by

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

where p_k is the number of cycles of length k in the permutation. The total number of conjugate classes is the number of partitions of n into integral summands. The quantity $b(\pi)$ is the redundancy, or number of member permutations in one conjugate class and is given by

$$b(\pi) = n! (1^{p_1} p_1! 2^{p_2} p_2! \dots n^{p_n} p_n!)^{-1}$$

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The quantity $d(\pi)$, known as the number of "degrees of freedom" connected with the permutation π , is defined by

$$d(\pi) = \sum_{h=1}^n \sum_{k=1}^n p_h p_k (h,k)$$

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

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

Davis has developed other formulas for enumerating specialized classes of relation:

Non-isomorphic reflexive (or irreflexive) relations

$$\text{ref}_n = \frac{1}{n!} \sum_{\pi} b(\pi) 2^{d_{\text{ref}}(\pi)}$$

$$d_{\text{ref}}(\pi) = d(\pi) - \sum_{k=1}^n p_k$$

Non-isomorphic symmetric relations

$$\text{sym}_n = \frac{1}{n!} \sum_{\pi} b(\pi) 2^{d_{\text{sym}}(\pi)}$$

$$d_{\text{sym}}(\pi) = \sum_{k=1}^n p_k \left\{ \left[\frac{k}{2} \right] + 1 + k(p_k-1)/2 \right\}$$

$$+ \sum_{h < k} p_h p_k (h,k)$$

$\left[\frac{k}{2} \right]$ = greatest integer function

Nonisomorphic irreflexive (or reflexive) symmetric relations

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$$\text{irs}_n = \frac{1}{n!} \sum_{\pi} b(\pi) 2^{d_{\text{irs}}(\pi)}$$

$$d_{\text{irs}}(\pi) = d_{\text{sym}} - \sum_{k=1}^n p_k$$

Non-isomorphic anti-symmetric relations

$$\text{asym}_n = \frac{1}{n!} \sum_{\pi} b(\pi) 3^{d_{\text{asym}}(\pi)}$$

$$d_{\text{asym}}(\pi) = \sum_{k=1}^n p_k \left\{ \left[\frac{k-1}{2} \right] + k(p_k-1)/2 \right\}$$

$$+ \sum_{h < k} p_h p_k (h,k)$$

Incidentally, note that ref_n is the number of directed graphs on n nodes and irs_n is the number of non-directed graphs.

All these formulas have been evaluated for n ranging up to 16 and the values are given in the accompanying tables. Asymptotic Formulae - Inspection of the various enumeration formulae given above shows that the dominant contribution to the total number of structures is due to just one of the partitions. This partition is the one consisting of n 1-cycles and corresponds to the identity transform of the group of transforms of the incidence matrix. Taking this term from each of the formulas we have

$$\text{str}_n^2 \sim 2^{n^2}/n!$$

$$\text{ref}_n \sim 2^{n(n-1)}/n!$$

$$\text{sym}_n \sim 2^{(n+1)^2/2}/n!$$

$$\text{irs}_n \sim 2^{n(n-1)/2}/n!$$

$$\text{asym}_n \sim 3^{n(n-1)/2}/n!$$

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To show the accuracy of these approximations, we give Table VII as a representative table. It appears that the asymptotic formulae are good to about one per cent if the true structure number is of the order of 10^{10} and are (naturally) better for larger structure numbers.

M. Douglas McIlroy

References:

- [1] R. L. Davis, Proc. Am. Math. Soc. 4(1953) 486
- [2] M. D. McIlroy, Machine Methods of Computation and Numerical Analysis, Quarterly Progress Report No. 15 (1955) p. 10

TABLE I Numbers of Structures of Relationships

n	all structures str _n	reflexive ref _n	symmetric sym _n	irreflexive symmetric irs _n	asymmetric asym _n
1	2	1	2	1	1
2	10	3	6	2	2
3	104	16	20	4	7
4	3044	218	90	11	42
5	$2.9197 \cdot 10^5$	9608	544	34	582
6	$9.6929 \cdot 10^7$	$1.5409 \cdot 10^6$	5096	156	21480
7	$1.1228 \cdot 10^{11}$	$8.8203 \cdot 10^8$	79264	1044	$2.1423 \cdot 10^6$
8	$4.5830 \cdot 10^{14}$	$1.7934 \cdot 10^{12}$	$2.2086 \cdot 10^6$	12346	$5.7502 \cdot 10^8$
9	$6.6666 \cdot 10^{18}$	$1.3028 \cdot 10^{16}$	$1.1374 \cdot 10^8$	$2.7467 \cdot 10^5$	$4.1594 \cdot 10^{11}$
10	$3.4939 \cdot 10^{23}$	$3.4126 \cdot 10^{20}$	$1.0926 \cdot 10^{10}$	$1.2005 \cdot 10^7$	$8.1601 \cdot 10^{14}$
11	$6.6603 \cdot 10^{28}$	$3.2523 \cdot 10^{25}$	$1.9564 \cdot 10^{12}$	$1.0190 \cdot 10^9$	$4.3744 \cdot 10^{18}$
12	$4.6557 \cdot 10^{34}$	$1.1367 \cdot 10^{31}$	$6.5234 \cdot 10^{14}$	$1.6509 \cdot 10^{11}$	$6.4540 \cdot 10^{22}$
13	$9.0169 \cdot 10^{40}$	$1.4669 \cdot 10^{37}$	$4.0540 \cdot 10^{17}$	$5.0502 \cdot 10^{13}$	$2.6378 \cdot 10^{27}$
14	$1.1521 \cdot 10^{48}$	$7.0316 \cdot 10^{43}$	$4.7057 \cdot 10^{20}$	$2.9054 \cdot 10^{16}$	$3.0037 \cdot 10^{32}$
15	$4.1233 \cdot 10^{55}$	$1.2583 \cdot 10^{51}$	$1.0231 \cdot 10^{24}$	$3.1426 \cdot 10^{19}$	$9.5773 \cdot 10^{37}$
16	$5.5343 \cdot 10^{63}$	$8.4446 \cdot 10^{58}$	$4.1788 \cdot 10^{27}$	$6.4001 \cdot 10^{22}$	$8.5888 \cdot 10^{43}$

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TABLE II Numbers of Structures of Dyadic Relations

n	str _n		
1			2
2			10
3			104
4			3044
5	2		91968
6		969	28992
7	11	22829	08928
8		45829	71000
9	6666	62157	21539
10			3493
11	90545	49349	98391
12			6660
13	85078	18075	85386
14			45648
15	89066	03112	66511
16	901685	91267	11300
17			76041
18	19117	62528	96061
19			48096
20			1152
21	57604	74157	55389
22			34617
23	43236	77230	31424
24			28672
25	4	12334	41401
26			68606
27	79295	18834	69376
28			48648
29	20973	59863	65854
30			35136
31			5534
32	25727	62971	20722
33			05192
34	57533	09620	02145
35			19348
36	89642	93721	27245
37			80352

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TABLE III Numbers of Structures of Reflexive (or irreflexive) Dyadic Relations

n				ref _n
1				1
2				3
3				16
4				218
5				9608
6			15	40944
7			8820	33440
8		179	33591	92848
9	13	02795	68243	99552
10	341260	43195	29725	80352
11			3	25229
	09385	05588	61111	97440
12		11	36674	54308
	25400	57443	38940	04224
13	146	69085	69271	29298
	69037	09607	53162	20928
14				7031
	56566	15234	99952	13855
	06555	97990	40912	17920
15		12	58345	26155
	04488	67281	04228	58105
	99188	12349	03206	83008
16	8444	60738	34225	80541
	87807	17815	32315	89171
	86915	03432	37883	67872

GRADUATE SCHOOL RESEARCH

TABLE IV Numbers of Structures of Symmetric Dyadic Relations

n				sym _n
1				2
2				6
3				20
4				90
5				544
6				5096
7				79264
8			22	08612
9			1137	43760
10			1	09262
11			195	63634
12			65233	50845
13			405	40227
14		4	70568	64216
15	10230	63423	47118	94310
16	41788492	03082	02323	60582
				29792

GRADUATE SCHOOL RESEARCH

TABLE V Numbers of Structures of Irreflexive (or reflexive) Symmetric Dyadic Relations

n	irs _n			
1				1
2				2
3				4
4				11
5				34
6				156
7				1044
8				12346
9		2		74668
10		120		05168
11		10189		97864
12		16	50911	72592
13		5050	20313	67952
14		29	05415	56572
15		31426	48596	98043
16	640	01015	70452	75578
				94928

GRADUATE SCHOOL RESEARCH

TABLE VI Numbers of Structures of Antisymmetric Dyadic Relations

n	asym _n			
1				1
2				2
3				7
4				42
5				582
6				21480
7			21	42288
8			5750	16219
9		41	59392	43032
10		81600	74490	11040
11	4374	40620	99707	47314
12				645
	39836	93872	07497	39356
13			263	77967
	35571	22500	90533	73136
14		300	36589	61589
	80530	05349	84908	93399
15	957	72686	34898	11549
	49990	83757	92075	81003
16				8588
	84182	49161	16546	12893
	38402	27902	32471	44414

GRADUATE SCHOOL RESEARCH

TABLE VII Comparison of Asymptotic Structure Formulae with True Formulae

	n = 7		n = 10		n = 15	
	approx. value	true value	approx. value	true value	approx. value	true value
str _n ²	1.117 10 ¹¹	1.123 10 ¹¹	3.493 10 ²³	3.494 10 ²³	4.123 10 ⁵⁵	4.123 10 ⁵⁵
ref _n			3.411 10 ²⁰	3.413 10 ²⁰	1.258 10 ⁵¹	1.258 10 ⁵¹
sym _n			.993 10 ¹⁰	1.093 10 ¹⁰	1.016 10 ²⁴	1.023 10 ²⁴
irs _n			.970 10 ⁷	1.201 10 ⁷	3.102 10 ¹⁹	3.143 10 ¹⁹
asym _n			8.140 10 ¹⁴	8.160 10 ¹⁴	9.577 10 ³⁷	9.577 10 ³⁷

PART II

Project Whirlwind

1. REVIEW AND PROBLEM INDEX

This report covers the specific period of June 13, 1955 to September 18, 1955. During this time, 94 problems made use of 337.3 hours of the 562.2 hours of Whirlwind I computer time allocated to the Scientific and Engineering Computations (S&EC) Group. The remaining 224.9 hours of the allocated time were used for terminal equipment testing and calibration, demonstrations, tape conversions for Lincoln Laboratory, and various inter-run operations not logged to specific problems.

These problems cover some 22 fields of applications. The results of 18 of the problems have been or will be included in academic theses. Of these, 12 represent doctoral theses, 1 engineering, 4 master's, and 1 bachelor's. Twenty-one of the problems have originated from research projects sponsored at M.I.T. by the Office of Naval Research.

Two tables are provided as an index to the problems for which progress reports have been submitted. In the first table the problems are arranged according to the field of application, and the source and the amount of time used on WWI is given. In Table 2-II the problems are listed according to the principal mathematical problem involved in each. In each table, the letter after the problem number indicates whether the problem is for academic credit and whether it is sponsored. The code is explained on page 28.

PROBLEM INDEX

Field	Description	Problem Number	Min. of Wkt Time	Supervisor or Programmer
Aeronautical Engineering	Transient response of aircraft structures to aerodynamic heating	236 C.	368.7	L. Schmidt
	Horizontal stabilizer modes, shapes, frequencies	277 C.	39.2	K. Wetmore
Aeroelastic and Structures Research Laboratory	Transient temperature of a box type beam	179 C.	45.6	L. Schmidt
	Factoring high order polynomials	314 C.	20.6	V. Howard
Aerophysics Research Group	Trajectory calculations for a rocket during powered flight	310 C.	60.5	J. Frizze
Building Construction Department	Partially continuous wooden beams	307	11.8	M. Weinstein
Business and Eng. Administration	Numerically controlled milling machine turbine blade	267 B.	190.5	G. Bromfield
Chemical Engineering	Transients in distillation columns	241 B.N.	322.3	S. Davis
	Calculations for the MIT reactor	260 A.	1807.1	M. Troost
	Heat transfer in turbulent flow	299 C.	373.4	A. Turano
	Critical mass calculations for cylindrical geometry	270 B.	499.9	J. Powell
Civil Engineering	Prediction of chromatographic separations	303 C.	474.8	J. Fischer
	Dynamic buckling	291 B.	74.4	R. Jones
Dynamic Analysis and Control Laboratory	Dynamic analysis of an aircraft interceptor	278 C.	174.5	K. Kavanagh
Electrical Engineering	Optimization of alternator control system	264 C.	87.7	J. Dennis
	Evaluation of a beam splitting technique	271 B.	218.2	F. Engel
Geology and Geophysics	Geophysical data analysis	106 C.	262.0	S. Simpson
	Fourier synthesis for crystal structures	261 C.	372.9	M. Rueger
Hydrodynamics Laboratory	Solitary wave generating cam	111 N.	122.1	J. Housley
Instrumentation Laboratory	Guidance and control	239 C.	234.9	J. Laning
	Data reduction for X-1 fire control	244 C.	7.4	J. Stark
	System analysis	246 C.	109.1	W. Kehl
Lincoln Laboratory	Eigenvalue problem for propagation of electromagnetic waves	193 L.	223.2	H. Dwight
	Ionosphere computation	275 L.	3049.2	D. Brennan
	General Raydist solution	272 L.	426.2	M. Huttenberg
	Tropospheric propagation	300 L.	282.1	H. Dwight
	Error analysis	112 L.	252.8	I. Shapiro
	Radar correlation	316 L.	32.9	M. Weinstein
Mechanics, Engineering	Flow of compressible fluids (aerothermopressor)	120 B.N.	837.0	A. Erickson
	Laminar boundary layer of a steady, compressible flow in the entrance region of a tube	199 N.	110.3	T. Toong
Meteorology Department	Synoptic climatology	155 N.	246.9	E. Kelley
	Computations of the fields of vertical velocity and horizontal divergence	224 N.	405.3	J. Austin
	Investigation of the vorticity field in the general circulation of the atmosphere	226 D.	382.6	R. Pfeffer
	Correlation function	280 B.	92.5	F. Hanna
Naval Supersonic Laboratory	Spectral analysis of atmospheric data	308 D.	43.9	H. Salzman
	Diffusion boundary layer	297 B.	371.4	J. Baron
Physics Department	Supersonic nozzle design	307 C.	39.1	J. Baron
	Self-consistent molecular orbital	144 N.	60.9	R. Nesbet
Miscellaneous	An augmented plane wave method as applied to sodium	194 B.N.	277.6	M. Saffren
	Exchange integrals between real Slater orbitals	204 N.	14.7	F. Merryman of Univ. of Chicago
	Transformation of integrals for diatomic molecules	218 N.	61.1	R. Nesbet
	Neutron-deuteron scattering	225 B.N.	171.4	L. Sartori
	Atomic integrals	234 N.	22.4	R. Nesbet
	Theory of neutron reactions	245 N.	1062.3	E. Campbell
	Application of the APW method to body- and face-centered iron	253 N.	163.0	J. Wood
	Energy levels of diatomic hydrides	260 N.	218.7	A. Freeman
	Evaluation of two-center molecular integrals	262 N.	375.2	H. Aghajanian
	Electron diffusion in an electromagnetic field	265 L.	81.6	D. Arden
	Analysis of air shower data	273 N.	193.2	G. Clark
	Multiple scattering of waves from a spatial array of spherical scatterers	274 N.	81.8	M. Karakashian
	Energy levels of diatomic hydrides L ₁ H	278 N.	411.9	G. Koster
	Augmented plane wave method as applied to crystal chromium	285 N.	52.9	M. Saffren
	Atomic wave functions	288 W.	806.7	R. Nesbet
	Electronic energy of the helium molecular ion	298 A.	246.6	B. Moiseiwitsch
	Relativistic atomic wavefunctions	304 N.	1054.4	C. Schwartz
Pure and impure KCl crystal	309 B.N.	36.5	L. Howland	
Data reduction program, polynomial fitting	426 C.	918.3	D. Ross	
Subroutines for the numerically controlled milling machine	132 D.	74.3	J.H. Runyon	
Miscellaneous	Comprehensive system of service routines	100.	2084.2	F. Helwig
	S & EC subroutine study	141.	978.9	S & EC Group
	Ultrasonic delay lines	212 C.	80.2	R. Bishop
	Comparison of simplex and relaxation methods in linear programming	219.	268.1	E. Baliffs
	Whirlwind I - SNA 1103 translation program	225 C.	336.9	J. Frankovich
	Course 6.2	305 B.	54.9	W. Eccles
	Frequency analysis of aperiodic functions	305 A.	91.9	J. Roseman
	Routines for course 6.001	313 D.	32.8	A. Siegel

Table 2-I Current Problems Arranged According to Field of Application

PROBLEM INDEX

Mathematical Problem	Procedure	Problem Number	
1. Matrix algebras and equations	Matrix multiplication, addition, diagonalization	144 N.	
	Orthogonalization	213 N.	
	Root of a determinantal equation	266 A.	
	Linear equations	270 B.	
	Simultaneous equations	277 C.	
	Eigenvalues	278 W.	
	Eigenvalues	285 N.	
	Eigenvalues	288 N.	
	Inversion	312 L.	
	Iteration		
2. Ordinary differential equations	Seven nonlinear first order	120 B.N.	
	System	199 N.	
	Set of first order equations	239 C.	
	Set of nonlinear first order	241 B.N.	
	Wave equation	245 N.	
	Set of eight first order	258 C.	
	Second order	259 N.	
	System of ordinary differential equations	291 B.	
	Nonlinear differential equations	296 C.	
	Second order	297 B.	
Second order nonlinear differential equations	310 C.		
3. Partial differential equations	Second order parabolic	236 C.	
	First order system	224 N.	
	First order system	226 D.	
	Second order	299 C.	
	Simultaneous partial differential equations	303 B.	
	Second order hyperbolic partial	379 C.	
	4. Integration	Integral evaluation	204 N.
		Stationary point of a variational	225 B.N.
		Overlap integrals	260 N.
		Integration	278 N.
Integral transformation		234 N.	
Overlap integral		262 N.	
Integration		304 A.	
Integrals		312 L.	
Fresnel integral		309 B.	
Conversion power series with a complex argument		300 L.	
5. Statistics	Multiple time series	106 C.	
	Calculation of the coefficients of a multiple regression system	155 N.	
	Multiple time series	259 L.	
	Maximum likelihood estimation	271 B.	
6. Transcendental equations	Multiple time series	280 B.	
	Nonlinear equations	264 C.	
	Nonlinear equations	272 L.	
	Curve fitting	275 N.	
7. Data reduction	Data reduction	126 C.	
	Surface fitting	267 B.	
	Miss distribution	244 C.	
	Polynomial fitting, etc.		
8. Group theory	Polynomial fitting, etc.	264 C.	
	Arithmetic operations	244 C.	
9. Complex algebra	Machine generation	194 B.N.	
	Complex roots and function evaluation	193 L.	
10. Fourier series	Iteration		
	Fourier synthesis	261 C.	
	Summing series	274 N.	
11. Linear programming	Fourier synthesis	306 D.	
	Linear programming	219	
	Linear programming	316 L.	
12. Factorization of Polynomials	Simplex method and relaxation method	216 C.	
	Simplex method and relaxation method	314 C.	
	Simplex method and relaxation method	307 C.	
13. Algebraic equations	Hitchcock's method		
	Newton-Raphson		

Table 2-II Current Problems Arranged According to the Mathematics Involved

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 (MMC) Group have been omitted from Section 2.2 of Part II to avoid duplication of Part I. For reference purposes, a list of the MMC Group problems appears on page 68.

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

- A implies the problem is NOT for academic credit, is UNsponsored.
- B implies the problem IS for academic credit, is UNsponsored.
- C implies the problem is NOT for academic credit, IS sponsored.
- D implies the problem IS for academic credit, IS sponsored.
- N implies the problem is sponsored by the Office of Naval Research.
- L implies the problem is sponsored by Lincoln Laboratory.

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

WHIRLWIND CODING AND APPLICATIONS

2.2 Problems Being Solved

100. COMPREHENSIVE SYSTEM OF SERVICE ROUTINES

The modifications proposed in the preceding Summary Report were made and tested during the past quarter and are now part of the working system.

Work is presently proceeding on a manual which will describe in some detail the structure of the comprehensive system.

F. C. Helwig
Digital Computer Laboratory

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 with the separation of "reflections" from background interference on these records. More complete descriptions of the problem and the approaches used are contained in the Digital Computer Laboratory Biweekly Report of June 15, 1953, and in "Detection of Reflections on Seismic Records by Linear Operators". (Wadsworth, Robinson, Bryan, and Hurley--GEOPHYSICS, Vol. 18, No. 3, July 1953).

The reader is referred to the March 25, 1955 quarterly report (Summary Report No. 41) for our recent approaches to the problem. During the last quarter we have concentrated on the following problem: the examination of a split spread multitrace seismogram for possible reflection signals, where the time position of the signal on each trace may vary due to both dip of reflector and finite curvature of the wave front, and the conversion of these results directly into structural information about the earth.

A program which has been developed for this purpose averages, for each small increment of time, cross-correlations across the record, along curves on which we would expect a reflection to fall for various trial dip angles, according to any given velocity function. (Actually it averages along two straight line segments, one on the upper half arc, one on the lower half, which represent the chords of the actual reflection curve arc.) For each increment the program then finds that dip angle which maximizes this average, prints out this angle and the maximum, converts the center time of the increment to an elevation and prints this elevation.

The program has been checked out and is now being run on actual records with different values of the averaging-length and trial step-out spread parameters. The results are very encouraging.

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.

Programmers during the summer have been S. Simpson, S. Treitel, and D. Pink, who are all associated with the M.I.T. Department of Geology and Geophysics.

S. M. Simpson, Jr.
Geology and Geophysics

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 cooling of the stream. The cooling of the hot gas is accomplished by evaporation of liquid water which is 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. This duct is 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 the 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 number of computations were made using the new Whirlwind program for the aerothermopressor (described in the Quarterly Report of March 24, 1955, No. 41). The computations can be divided into three groups:

1. Theoretical calculations to compare with experimental results from the aerothermopressor being tested in the Gas Turbine Laboratory. These comparisons are included in an Sc. D. thesis by Arthur A. Powle entitled "An Experimental Investigation of an Aerothermopressor Having a Gas Flow Capacity of 25 Pounds Per Second". A typical example of such a comparison (Figure 19 from the thesis) is included with this report.
2. A theoretical investigation of the desirability of having supersonic gas velocities at the plane of water injection. Calculations indicate performance of the aerothermopressor improves when supersonic velocities are used. This result, however, does not include the effect of increased friction upstream of the water injection plane.
3. A study of conical diffusers with different angles of divergence in order to design a better experimental aerothermopressor for testing in the Gas Turbine Laboratory.

The aerothermopressor program is being carried out at M.I.T. under the sponsorship of the Office of Naval Research and is being directed by Professor Ascher H. Shapiro of the Department of Mechanical Engineering. The theoretical aspects of the problem treated by Whirlwind I were programmed by Bruce D. Gavril and are now being carried out by Alve J. Erickson.

A. J. Erickson
Mechanical Engineering

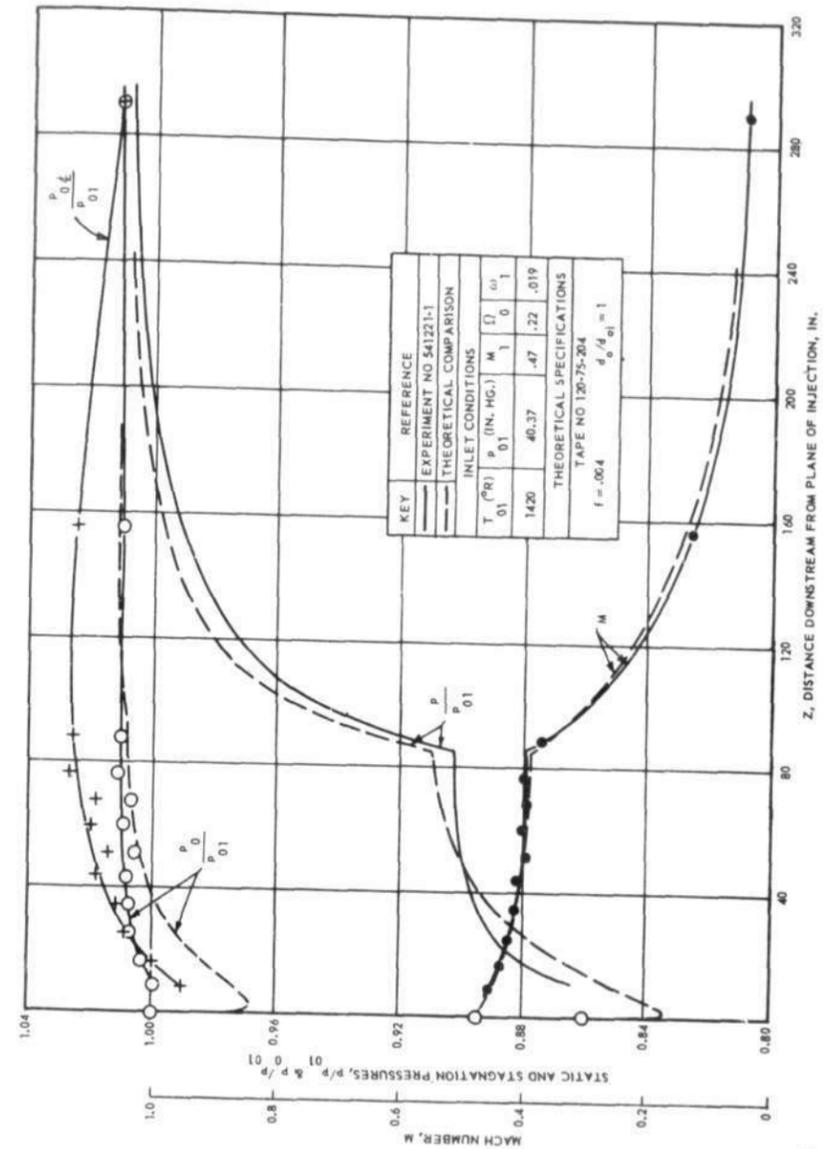


FIG. 19 COMPARISON OF THEORETICAL AND EXPERIMENTAL RESULTS

WHIRLWIND CODING AND APPLICATIONS

126 D. DATA REDUCTION

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

The nature of the problem requires 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 modifications. For this reason extensive use is made of output oscilloscopes so that the computer can communicate with the human, and manual intervention registers so that the human can communicate with the computer in terms of broad ideas, while the computer is running, and have the computer program translate these ideas into the detailed steps necessary for program modification to conform to the human operator's decision. The program which does this translation and modification is called the Manual Intervention Program (MIV). The most recent version of the prototype data-reduction program is called the Basic Evaluation Program.

Most of the computer time during this quarter was used in testing and modifying the WWI-1103 Translation Program described in Problem 255. Three programs were written in the ERA 1103 code for translation by this program. Two of these programs were written to test the oscilloscope display unit attached to the Air Force Armament Center 1103 Computer at Eglin Air Force Base, Florida. One is a Scope Flexowriter Program which writes characters on the scope corresponding to a Flexo tape read into the computer. The other program is the Mouse Program which simulates a mouse solving a 16 x 16 maze with the successive steps drawn on the scope by the program. The third program, A Basic Input Translation Program for the ERA 1103 Computer, is a companion to the program of Problem 256 except that symbolic addresses are not allowed. This program will be used to make corrections to programs translated on WWI at the 1103 site.

The Basic Evaluation Program has again been rewritten to incorporate still newer versions of the equations and to simplify the organization of storage locations. The Part I Program has also been again rewritten using many preset parameters to allow additional inputs and outputs in arbitrary formats. The sine and cosine routines have also been modified to use local Taylor expansions to greatly increase the speed of the program at no cost in accuracy. The program chooses the Taylor Expansion if it will give sufficient accuracy, but chooses the library subroutine otherwise, and uses the results to generate a new Taylor expansion about the new point for use on succeeding steps.

The Manual Intervention Program (MIV) has gone through several new revisions in efforts to generate a system which will allow, essentially, programming with programs while the computer is in operation. The Director Tape Program has been modified under Problem 100 so that the new system can incorporate all of the Comprehensive System without restriction. Logging and Editing Programs are being written by S & EC group programmers so that every action taken or display seen can be permanently logged in an easily understood form.

D. T. Ross
Servomechanisms Laboratory

WHIRLWIND CODING AND APPLICATIONS

132 D. SUBROUTINES FOR THE NUMERICALLY CONTROLLED MILLING MACHINE

The following work was done during the past quarter under Problem 132:

1. A completed punched paper tape was used to cut a machine cam using the Numerically-Controlled Milling Machine. This work was submitted by John Runyon in a thesis report.
2. A completed punched paper tape was used to cut out a profile cam for Chandler-Evans Corporation, Hartford, Connecticut. This work was also submitted by John Runyon in a thesis report.
3. A third program was not completed. However, the Hydromatic Laboratory under the sponsorship of the Navy has resumed work on this program.

Problem 132 is now terminated with regard to Whirlwind I.

T. Nagle
Servomechanisms Laboratory

141 SUBROUTINE STUDY OF THE SCIENTIFIC AND ENGINEERING COMPUTATIONS (S & EC) GROUP

1. Factorization of Polynomials

CS II routines for factoring nth degree polynomials have been coded and tested, and have solved several tenth degree polynomials arising from physical problems. The tapes are on file, and their use is described in DCL-94-1. Research is continuing on numerical factorization methods.

A CS II routine now almost ready for use will express functions given as long Taylor series in terms of sums of Tschebyscheff polynomials $T_n(x)$. This type of expression minimizes the maximum error when the series representing a function must be truncated. A measure of the truncation error will be given. A Digital Computer Laboratory memorandum describing the routine in detail is in preparation.

M. Jacobs

2. Iterative Solutions

A preliminary routine has been developed for iterative solution of linear systems. The method is particularly suited for use with large matrices, most of whose elements are zero, a type encountered commonly in network analysis or discretized elliptic partial differential equations. Further, such matrices are commonly loaded along the main diagonal. This characteristic, too, is capitalized on by the iterative process.

The iterative approach to a solution has two advantages. In the first place, only enough storage registers need be provided to take care of the non-zero elements in the matrix, whereas reduction processes such as Gauss-Jordan or Crout can not so profit from the character of the matrix. Secondly, initial data are used at each stage of the iteration, obviating the necessity of carrying large numbers of superfluous digits in order to overcome round-off. One can expect, though, that iteration will be very slow in convergence for large systems and this factor must be weighed against the advantages.

In respect to time, the routine does not compare favorably with Crout's method for small matrices, but near the limiting size (28 x 28) of matrices which can be handled in core-memory by a Crout routine, the iterative routine becomes competitive. It is expected that the latter method will in general take a time roughly proportional to n^2 while Crout's method takes a time proportional to n^3 . In storage requirements, the iterative routine is limited only by the number of off-diagonal elements in the matrix. A 100 x 100 symmetric matrix with 400 off-diagonal elements can be handled in core storage, using two-register arithmetic.

The Jacobi iteration was chosen as that method which best takes advantage of all the characteristics of matrices of the type which was confronted. The method and the routine are described in some detail in memorandum DCL-101.

M. D. McIlroy

3. Histogram Plotter

A general routine for plotting histograms on the oscilloscope face has been written and tested. After 6 program parameters are given, it plots and calibrates axes and plots the histogram from a series of registers containing Whirlwind I integers. The routine takes 233 registers and refers to a decimal integer display routine occupying 86 registers.

M. D. McIlroy

4. FU4A RAPID SINE-COSINE

A new version of the (30-J,J) sine-cosine subroutine is available. The operating time is equivalent to 18 or 19 interpreted instructions as opposed to upwards of 31 interpreted instructions for the previous FU 4 subroutine. Accuracy of this routine is exactly the same as that of FU 4. Space requirement is 78 registers plus 4 registers of temporary storage.

M. D. McIlroy

5. OS4 SCOPE MRA DECIMAL FORMAT

This routine displays normalized generalized decimal numbers from the interpreted Multiple Register Accumulator (MRA) on the scope in any rectangular array that does not overreach a basic 40 x 40 grid on the scope face. Positioning of numbers proceeds sequentially either by row or by column. The format pattern may be changed at will by the programmer by means of program parameters. This routine occupies 248 registers and uses 2 registers of temporary storage.

M. D. McIlroy

6. OS5 SCOPE MRA DECIMAL OUTPUT

Basically, this routine is identical to OS4, except that the format is fixed by preset parameters. OS5 occupies 205 registers and uses 3 registers of temporary storage.

M. D. McIlroy

7. Printout Subroutines

The following subroutines have been added to the subroutine library:

- a. OD 6 Delayed Single Length Decimal Integer Print
- b. OD 7 Delayed Octal Print
- c. OD 8 Single Register Block Print (program parameters)
- d. OD 9 Single Register Block Print (preset parameters)
- e. OD 10 (30-J,J) Decimal CS Print
- f. OD 11 (30,15) Decimal Print (CS or WW)
- g. OD 12 CS (30-J,J) Block Print (preset parameters)
- h. OD 13 CS (30-J,J) Block Print (program parameters)

Four of the delayed output routines (OD 6, OD 7, OD 10, and OD 11) print out numbers. The first three are rewrites of OD 3, OD 5, and OD 2, respectively. In each case they are shorter than the original. All four routines have been written so that they may be used with the remaining four (OD 8, OD 9, OD 12, and OD 13) for printing out blocks of numbers from high-speed storage without magnetic tape stoppage between numbers. The number printout routines have banks of entrance blocks providing various terminating characters. These banks lie at the end of the routines. Unused entrance blocks can be deleted, thus shortening the routine.

Two of the four block print routines provide for printing single register numbers. The other two are for double register numbers. The parameters for the block routines are:

- (1) The initial high-speed address of the block of numbers to be printed.

- (2) The address of the subroutine printing the number (OD 6, 7, 10, or 11).
- (3) The number of numbers in the block.
- (4) The number of numbers per line.
- (5) The terminating character between numbers on a line.

Of each pair of block routines, one has this information in preset parameter form, while the other has it in program parameter form. The preset parameter routines are shorter but less flexible.

OD 11 is modeled after the FA PM printout routine. It provides more correct digits than any previous LSR output. For numbers with exponents of large magnitude it is the most rapid routine to date and it will successfully print numbers with binary exponents up to $\pm 2^{12}$.

R. Watson

8. FU RAPID SQUARE ROOT

FU 8 is a square root routine which takes, as its first approximation, the first three terms of the Tschebyscheff series and then does one iteration by Newton's method. This routine takes 5 milliseconds as against 30 for FU 2, and it is one octal digit less accurate.

R. Watson

144 N. SELF-CONSISTENT MOLECULAR ORBITAL

Several revisions were made in subroutines developed under this problem in connection with the work on Problem 288.

R. K. Nesbet
Solid State and Molecular Theory
Group

155 N. SYNOPTIC CLIMATOLOGY

During the past quarterly period, two phases of the Synoptic Climatology Project have utilized Whirlwind I. The method, essentially one of multiple linear regression, has been developed and improved over the past two years, mainly by Dr. Thomas P. Malone and Mr. Robert G. Miller.

The first phase has dealt with the prediction of 24 hour precipitation amount and duration at Boston, Massachusetts. The analysis has been extended to include the effects of the upper level circulation and moisture distribution, in addition to the sea-level pressure pattern on the variability of rainfall.

In this study two basic operations are involved: 1) representation of the fields of certain continuous variables (e.g. pressure, moisture) in terms of series of coefficients of orthogonal polynomials; and 2) matrix solution and inversion. Programs have been written previously by Mr. Robert G. Miller to accomplish both of these operations and only slight modifications were necessary to fit them to the present study.

As an extension of the above, it is planned to apply essentially the same methods to the specification and prediction of 5-day mean precipitation over the entire United States.

The second phase has dealt with the specification, prediction, and verification of forecasts of 5-day mean temperature anomalies at Atlanta, Ga.; Bismark, N. D.; Indianapolis, Ind.; Little Rock, Ark; and Portland, Me. Also, the specification and prediction of 5-day precipitation totals at the same stations has been handled in this study. The prediction parameters used are standardized correlation coefficients between 700 mb. 5-day mean height anomalies and the elements of Tschebyscheff orthogonal polynomials. This phase of the project is nearing completion and it is hoped to combine all of these results in a scientific report.

Work is being performed by Mr. W. D. Sellers on the first phase, and by Miss Elizabeth A. Kelley on the second phase, both under the supervision of Professor Henry G. Houghton, and Dr. Edward N. Lorenz, Department of Meteorology.

W. D. Sellers
Meteorology

179 C. TRANSIENT TEMPERATURE OF A BOX-TYPE BEAM

In Summary Report No. 39 a program for computing the transient temperature and stress response at one cross section in a simple thin walled beam, exposed on one surface to thermal radiation, was reported. During the past report period this program has been used to obtain transient temperature and stress responses for the same structure when exposed to various intensities of thermal radiation on one surface. These results are to be correlated with experimental work recently conducted by Mr. S. J. Engel of the Aeroelastic and Structures Research Laboratory.

Lucien A. Schmit
Aeroelastic and Structures
Research Laboratory

193 L. EIGENVALUE PROBLEM FOR PROPAGATION OF ELECTROMAGNETIC WAVES

The previous report on this problem applies at the present time. A set of practical results which can be compared with the experimental results will be obtained in the near future.

H. B. Dwight
Lincoln Laboratory

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

Mr. M. Saffren of the Solid State and Molecular Theory Group continues to test the programs mentioned in the previous Summary Report.

It has been found that the matrix element generation routine which has been used is overly slow and largely inaccurate; therefore, a new routine is being written.

M. M. Saffren
Solid State and Molecular Theory
Group

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 to a stream of air flowing at supersonic speeds in a round tube, a theoretical investigation of the characteristics of the laminar boundary layer in the entrance region of the tube has been carried out. The boundary layer equations of continuity, momentum and energy are to be solved for specific entrance Mach numbers and thermal conditions at the tube wall.

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

Solutions of the first three sets of the differential equations for the case where the entrance Mach number is 2.8 and the tube wall is insulated were obtained with the new program using CS. The trial-and-error procedure set-up to find the correct initial conditions is satisfactory.

Programs are being prepared for the solution of the differential equations for the case where temperature dependence of the fluid viscosity and thermal conductivity is taken into consideration.

T. Y. Toong
Mechanical Engineering

204 N. EXCHANGE INTEGRALS BETWEEN REAL SLATER ORBITALS

As is usually reported the testing of this program continues. However, with the insertion of an adequate set of constants for a sufficiently accurate gaussian quadrature, the program has proved able to give satisfactory results. Thus, at this juncture, the program has fulfilled the projected specifications both as to mathematical procedure and programming accuracy. The testing that shall be continued will be primarily devoted to more extensive investigation of the complicated mathematical development, that is, of an order of magnitude larger than one amenable to hand computation.

The program that has been developed was envisioned as a step in the calculation of molecular wave functions, and while meaningful alone, has its primary use in this context. For this reason the projected succeeding step is a program designed to compute all of the integrals necessary to the computation of a molecule and organized to take careful account of the "computing weights" of each operation. This program should be forthcoming within the next year and will be described more fully in a later report.

P. Merryman
Laboratory of Molecular Structure
and Spectra
University of Chicago

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This problem is concerned with maximization of the reflection path aperture of a polygonal ultrasonic delay line.

The aperture of such a delay line is determined by the difference between the least ordinate of one set of points in a plane and the greatest ordinate of another set of points. Expressed symbolically we have two sets of ordinates

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The aperture then is given by $A = \min H_1^T - \max H_1^B$. The H_i , and hence, also A , are functions of the size, shape, and position of the polygon in a coordinate system. A , however, is independent of the position. The size, shape, and position are determined by the distances, R_j , of the facets from the origin and the angles which they make with the x-axis. These variables are given initial values, and then any new values are determined by changes, ΔR_j and d_j , from the old ones.

The equations for H_1^T and H_1^B are linear in the variables ΔR_j and are algebraic expressions of trigonometric functions of the d_j . The latter are quite linear over the small range for the d_j with which we are concerned, so that the approximate linear equations can be used to good advantage. We thus arrive at a set of equations

$$H_1^T = {}^0H_1^T + \sum_{j=0}^{n-1} a_{1j} \Delta R_j + \sum_{j=0}^{n-1} a'_{1j} d_j, \quad i=0, \dots, p$$

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where n = number of sides of the polygon. The matrices of coefficients $\{a_{1j}\}$, $\{a'_{1j}\}$, $\{b_{1j}\}$, $\{b'_{1j}\}$ are computed by a program on Whirlwind I as the initial step of the problem.

Since we want to maximize A with respect to only the shape of the polygon, we must impose other conditions on the variables. Also, certain physical requirements are made of the angles. Altogether, these lead to four other equations which the variables must satisfy and, in addition, if the polygon is symmetric, there are n more conditions. For each additional condition one variable is eliminated. This is done on Whirlwind as the second step of the problem, in addition to a transposition of the matrix and the addition of four variables needed in the linear program.

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M. M. Saffren
Solid State and Molecular Theory
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T. Y. Toong
Mechanical Engineering

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WHIRLWIND CODING AND APPLICATIONS

When these two steps have been completed, the problem is then reformulated. After elimination of variables to make the remaining ones independent, we have a set of variables u_j corresponding to the ΔR_j , and v_j corresponding to the σ_j and a set of linear inequalities, rather than equalities, for which we wish to maximize the quantity $\epsilon_1 + \epsilon_2 = A$:

$$\epsilon_1 - \sum c_{1j} u_j - \sum d_{1j} v_j \leq {}^T H_1, \quad 1=0, \dots, p$$

$$\epsilon_2 + \sum d_{1j} u_j + \sum d'_{1j} v_j \leq -{}^B H_1, \quad 1=0, \dots, p$$

We must make further substitutions, since the simplex method of linear programming is to be used, and this method requires that the variables and the constant part of the inequalities must be non-negative. The variables y_1 and y_2 are introduced for each u_j . We substitute a new variable $U_j = u_j + y_1$ and for each v_j we substitute a new variable $V_j = v_j + y_2$. To make the constants non-negative we merely add .5 to each of them, and now consider our problem to be the maximization of $\epsilon_1 + \epsilon_2 - 1 = A$. Since we know that H_1^T and $-H_1^B \geq -.5$ initially, this accomplishes our purpose. It will also come out in our solution that $-y_1 = \min u_j$ and $-y_2 = \min v_j$ so that U_j and V_j are non-negative.

An additional program is required after the linear program to reconvert the results back to the original variables. The output of the results may then be provided for and an iteration of the entire process may be set up in case the σ_j are large enough so that they no longer can be treated as linear variables.

The second step of this process actually requires two programs, one for the symmetric case and one for the non-symmetric case.

Since the first program requires a considerable quantity of data which can be determined from much less information, another program is to be used to compute the data, and also to change the parameters in the other programs to accommodate different polygons.

The first of the programs mentioned above, as well as the program for the symmetric case in the second step, have been written and checked, as has the linear programming routine. The latter, however, is under revision to take advantage of the new si instructions for the auxiliary drum. The program used in the fourth step has been written. Some work has been done on the program for the non-symmetric case in the second step which will be similar enough to the symmetric case as to give no trouble. The program for setting up data is not started but will not be complicated.

R. Bishop
Arenberg Laboratory

218 N. TRANSFORMATION OF INTEGRALS FOR DIATOMIC MOLECULES

Several revisions were made in subroutines developed under this problem in connection with the work on Problem No. 288.

R. K. Nesbet
Solid State and Molecular Theory
Group

219 COMPARISON OF SIMPLEX AND RELAXATION METHODS IN LINEAR PROGRAMMING

A program has been written to solve the classical transportation problem by the stepping stone method.

The transportation problem may be stated as follows: A company operates plants producing a commodity, the i^{th} of which can supply S_i units of the commodity. The company sells its production to n customers, the j^{th} of which desires D_j units of the commodity. The cost of manufacturing and transporting a unit of the commodity from plant i to customer j is C_{ij} . It is desired to find the number of units X_{ij} that should be shipped from each plant to each customer, in order to have the total cost of the operation be a minimum.

WHIRLWIND CODING AND APPLICATIONS

Thus the problem may be stated mathematically as

$$\text{minimize } C = \sum_{i,j} C_{ij} X_{ij} \quad (1)$$

subject to the constraints

$$\sum_j X_{ij} = D_j \quad (2)$$

$$\sum_i X_{ij} = S_i \quad (3)$$

$$X_{ij} \geq 0 \quad (4)$$

This is a special case of the general linear programming problem.

A set of X_{ij} which satisfies equations 2, 3, and 4 is called a feasible solution to the problem. If the set also minimizes C , it is an optimum feasible solution containing, in general, exactly $m+n-1$ non-zero X_{ij} .

The process of solution consists of

- 1) generating a feasible solution having exactly $m+n-1$ non-zero X_{ij} .
- 2) finding a zero X_{ij} which, if allowed to be positive, would yield a decrease in C . In the process of increasing this X_{ij} , one of the non-zero X_{ij} must go to zero in order that equations 2 and 3 remain satisfied. Thus the new feasible solution will again have exactly $m+n-1$ non-zero X_{ij} .

Step 2 is repeated until there are no zero X_{ij} which can be changed so as to reduce C . The set of X_{ij} is then an optimum feasible solution.

The Whirlwind program will handle problems for $m \leq 128$, $m+n \leq 400$, and $mn \leq 7000$. The program is presently in the final debugging stage.

In the next quarter debugging will be completed and the program will be put in convenient form for users. Production runs will be performed with a number of sets of data.

This work is being supervised by Associate Professor W. K. Linvill of the Electrical Engineering Department. Programmers are J. B. Dennis, Research Assistant, and W. J. Eccles, Teaching Assistant, in the Department of Electrical Engineering.

This project has been supported in part by a grant-in-aid from the Union Carbide and Carbon Corporation.

J. B. Dennis
Electrical Engineering

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

The nature of the problem has been presented in Project Whirlwind Summary Report No. 41. During this quarter the fields of vertical motion, horizontal divergence and vorticity were computed for eight consecutive 12-hour periods. No additional computations are planned until the Pressure Change Project of the Department of Meteorology has analyzed the results.

J. M. Austin
Meteorology

WHIRLWIND CODING AND APPLICATIONS

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

1. Description of Problem: The physical processes which are important in the maintenance of the general circulation of the atmosphere are being investigated with the aid of a two parameter, non-linear, quasi-geostrophic model of atmospheric flow. The model makes use of the vorticity equation and the first law of thermodynamics and incorporates effects of non-adiabatic temperature changes and friction as well as the vertical advection of vorticity and the transformation of horizontal vorticity into vertical vorticity. A spherical coordinate system with pressure as the vertical coordinate has been used in the derivation, and the model is being applied to the Northern Hemisphere from 15° N. to 80° N. latitude. The two parameters used to describe the flow are the 700 mb and 300 mb contour heights.

With the aid of the model described above it is planned to examine the role of various heating distributions in generating the gross features of the general circulation. These distributions are described in the initial report. (Quarterly Report for Project Whirlwind, Summary Report No. 42, Second Quarter, 1955). The equations of the model are also given in the initial report.

2. Numerical Procedures: An inverse matrix of a simple finite difference operator applied to 30 grid points has now been calculated. A solution involving the same simple operator has also been obtained by relaxation. The results are being compared in terms of accuracy and machine time used. It is planned to repeat the work for 60 grid points and extend the comparison. The program for calculating one group of non-homogeneous terms of the differential equations is nearly completely tested.

3. Progress and Future Plans: During the next quarter other matrices of 30th or 60th order will be inverted and the inverses will be multiplied by the sums of the non-homogeneous terms to obtain initial values for the thickness tendency. This quantity will be used in programs yet to be tested for equations used to determine initial values of vertical velocity and 700 mb height tendency.

If the relaxation program proves satisfactory, it may replace the matrix inversion program in determining the inverse of the finite difference operators used in the problem.

4. Personnel: This research is being carried out under the sponsorship of the Air Force Cambridge Research Center by the following persons:

Richard L. Pfeffer
Geophysics Research Directorate

Duane S. Cooley
Geophysics Research Directorate

Paulo Castillo
General Circulation Project, MIT

Kirk Bryan, Jr.
General Circulation Project, MIT

Messrs. Castillo, Bryan, and Cooley are writing the program for the problem. Mr. Martin Jacobs of the Digital Computer Laboratory has been assisting them.

D. S. Cooley
Meteorology

WHIRLWIND CODING AND APPLICATIONS

234 N. ATOMIC INTEGRALS

A program has been constructed which evaluates integrals of the type

$$[V_A]_{L_A} = \int_{d\tau} \frac{1}{|x-K|} \eta_A^*(x) \eta_B(x),$$

where

$$\eta_A = N_A r^{A+L_A} e^{-\lambda_A r} Y_{L_A}^m(\theta, \phi).$$

Here N_A is a normalization constant. These integrals are evaluated for arbitrary non-negative integers A and L_A and arbitrary positive values of λ_A . Results calculated with this program agree with hand calculations to between seven and eight significant decimals. Details of this program will be given in Quarterly Progress Report, Solid State and Molecular Theory Group, M.I.T., October 15, 1955.

R. K. Nesbet
Solid State and Molecular Theory
Group

236 C. TRANSIENT RESPONSE OF AIRCRAFT STRUCTURE TO AERODYNAMIC HEATING

The transient response of aircraft structures to aerodynamic heating was initiated on January 3, 1955, by L. A. Schmit of the M.I.T. Aeroelastic and Structures Research Laboratory. A program to compute the transient temperature and stress distributions in a structure simulating an aircraft wing has been written and run successfully. The partial differential equations of heat flow were solved by finite difference approximations similar to those reported in detail in the last Quarterly Progress Report. A more realistic flight history was incorporated in this program than in the thin plate or thin plate and web programs.

The results of this program are now being analyzed and several more runs are being planned.

H. Parechian
Aeroelastic and Structures Research
Laboratory

239 C. GUIDANCE AND CONTROL

No work was done on this problem during the past quarter that was not classified.

J. H. Laning, Jr.
Instrumentation Laboratory

241 B. N. TRANSIENTS IN CONTINUOUS DISTILLATION SYSTEMS

Additional programs have been written to study the transient behavior of an ideal model of a continuous distillation column. The study of two classes of problems has proceeded through the use of these programs:

- 1) A column at equilibrium operating under certain conditions is suddenly caused to go into a transient state by a sudden change in one or more of its operating conditions.
- 2) A column at equilibrium suddenly has its feed composition changed, and during its transient state the vapor-liquid ratios are adjusted at intervals so that the product compositions are prevented from fluctuating to any significant extent.

S. H. Davis, Jr.
Chemical Engineering

WHIRLWIND CODING AND APPLICATION

244 C. DATA REDUCTION FOR X-1 FIRE CONTROL

This problem is concerned with computing from gun fire control signals the distance by which fictitious projectiles miss an observed target. A brief description of the tape prepared for this problem is found in Summary Report No. 41 for the First Quarter, 1955. Since this tape may be used, with minor changes, in processing new data, this is to be considered a terminating report.

The problem was coded by Dr. J. M. Stark of the M.I.T. Instrumentation Laboratory. Results are classified information.

J. M. Stark
Instrumentation Laboratory

244 N. THEORY OF NEUTRON REACTIONS

In the Summary Progress Report No. 42, a master program was described which for any given x will find the cross sections for any range of x_0^c by the use of a suitable parameter tape.

Several logical errors have been uncovered and eliminated in this master program. There still remains a discrepancy between the cross-sections computed by this program and the known value for the particular case of a real square well. When this trouble is cleared up it is planned to proceed as indicated in the previous progress report.

E. Campbell
Joint Computing Group

253 N. APPLICATION OF THE A P W METHOD TO BODY-CENTERED AND FACE-CENTERED IRON

The energy band solutions for one-electron wave function in face-centered and body-centered iron is proceeding via the APW (augmented plane wave) method. (Ref. 1.) Having chosen an approximate crystal potential, the first step is the formation of the so-called 'Evs. E₀' curves. (Ref. 1,2.) These curves are currently being produced for the face-centered structure, using programs developed by Howarth and Saffren.

A program is being written which will form the electronic charge density from the one-electron wave functions.

J. H. Wood
Solid State and Molecular Theory
Group

References

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M. M. Saffren and J. C. Slater, Phys. Rev. 92, 1126 (1953).
2. D. J. Howarth, Phys. Rev. 99, 469 (1955).

256 C. WWI-1103 TRANSLATION PROGRAM

A version of the two-pass input translation program described in Summary Report No. 41 is operating satisfactorily on WWI. Problems coded for the ERA 1103 computer in the described mnemonic code can now be fed into WWI in the same automatic manner as CS flexo tapes with the resulting output being a machine-coded binary tape which can be read directly into an 1103. This procedure is being used now by Problem No. 126 programmers, who are making use of both WWI and the Air Force Armament Center 1103 computer at Eglin Air Force Base.

Some modifications have been made to the translation program during the past quarter to make the binary tapes more easily acceptable to the ERA photoelectric tape reader equipped 1103's. Many more changes have been made to improve the techniques used

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In such translation programs as well as to enlarge the vocabulary of the input language. A summary report on the program will be written in the next quarter.

J. M. Frankovich
Digital Computer Laboratory

256 D. DYNAMIC ANALYSIS OF AN AIRCRAFT INTERCEPTOR

During the past quarter, four solutions of this problem were run on Whirlwind I. The basic program consisted of a solution by the Gill method of eight nonlinear differential equations describing the motion of an aircraft. The current runs solved this basic program with certain changes in the original equations and in the input constants and functions. The modifications were ascertained by a study of the results of runs made in the previous quarters.

The completion of the present series of runs brings to an end the Whirlwind I phase of the problem. Results of this phase and of the analogue study completed on the M.I.T. Flight Simulator of the Dynamic Analysis and Control Laboratory will be described in D.A.C.L. Technical Report No. 95, September, 1955, and W.A.D.C. Technical Report No. 55-247, July, 1955, being written by engineers of the D.A.C. Laboratory and the Department of Aeronautical Engineering.

K. Kavanagh
Dynamic Analysis and Control
Laboratory

259 L. THE MEDIUM FREQUENCY IONOSPHERIC PROPAGATION STUDY

This problem was described in Summary Report No. 42. Data processing continued during the past quarter and is nearing completion.

D. G. Brennan
Lincoln Laboratory

260 N. ELECTRONIC ENERGY OF THE OH MOLECULE

Using the one- and two-electron (one- and two-center) integrals, calculated on Whirlwind I, the matrix elements for the calculation of energy have been computed following the Löwdin procedure for handling non-orthogonal functions. These are now being used to calculate the ground state energy of the OH molecule at the observed internuclear distance. The 10 x 10 secular equation is diagonalized on Whirlwind.

A whole new set of basic integrals is now being calculated at an internuclear distance larger than the observed one. This will serve as a check on the previous calculation and will determine the energy minimum of the E vs. r curve for the molecule.

A. J. Freeman
Solid State and Molecular Theory
Group

261 C. FOURIER SYNTHESIS FOR CRYSTAL STRUCTURES

The problem, which was first mentioned and described in Summary Report No. 42, was continued during this quarter. Particularly, the complete 3-dimensional Patterson function for Diglycinhydrochloride was computed by Whirlwind from which, at the moment, the 'minimum function' is being obtained. Further, the crystal structure of Bectolite was essentially solved, and progress was made towards the solution of Wollastonite.

Professor M. J. Buerger
Geology and Geophysics

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262 C. EVALUATION OF TWO-CENTER MOLECULAR INTEGRALS

The evaluation of two-center integrals between $1s$, $2s$, $2p$, and $2p\pi$ Slater orbitals is partly completed. Two hundred and forty hybrid integrals have been evaluated by the use of P. J. Corbató's κ -generation and numerical integration program. Also, one hundred and twenty exchange integrals have been evaluated by P. Merryman's exchange-integral program.

This problem was described in Summary Report No. 41.

H. A. Aghajanian
Solid State and Molecular
Theory Group

264 C. OPTIMIZATION OF ALTERNATOR CONTROL SYSTEM

In the last progress report for this problem, it was suggested that the problem of optimizing the design of a system could be phrased as a minimization problem. Part of the work completed in the past quarter consisted in coding a minimization procedure. The method of steepest descent appeared to be the only promising method. Although this method is available as a library subroutine, it is set up only for cases where expressions are available for the necessary derivatives. Since we wish our technique to be able to handle empirical functions such as magnetization curves, writing expressions for the derivatives is impractical. Therefore, a program was coded and successfully run which performs the method of steepest descent and uses difference techniques to evaluate the derivatives.

A scheme has been worked out to apply the steepest descent technique to the problem of minimizing a function of n variables subject to constraints. Coding of this scheme has not started yet, but will be undertaken during the next quarter. Personnel for this quarter were R. M. Saunders, Professor of Electrical Engineering (visiting), and J. B. Dennis and R. F. Newe, Research Assistants in Electrical Engineering.

The work reported here is under the sponsorship of the U. S. Air Force, Contract AF 33(616)2669, "Study of Aircraft A-C Generating and Voltage Regulating Systems."

J. B. Dennis
Electrical Engineering

265 L. ELECTRON DIFFUSION IN AN ELECTROMAGNETIC FIELD

Work on this problem was described in some detail in Summary Report No. 42.

On a subsequent set of parameter values it developed that a smaller interval size was required. Partial results were obtained for this set of parameters and the problem was terminated.

D. N. Arden
Digital Computer Laboratory

266 A. CALCULATIONS FOR THE MIT REACTOR

The program to calculate the reactor behavior for slow but sustained changes in reactivity was successfully finished. The method outlined in the last quarterly report was used.

A great number of data were obtained for subcritical and supercritical systems. A strong variation in the average neutron lifetime with ρ , the reactivity, and the amount of poison present, was found.

The method described in the last report to obtain a zero determinant worked only with the heavy-water-cooled reactors; in cases with light water the round-off errors became too large. Alternate methods are being investigated. All programming and

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coding was done by M. Troost.

This program is being carried out for the Nuclear Reactor Project.

M. Troost
Chemical Engineering

267 B. NUMERICALLY CONTROLLED MILLING MACHINE TURBINE BLADE

The airfoil portion of the jet engine turbine bucket used in this study is described by the coordinates of 272 points, the upper and lower boundaries of eight unequally spaced but parallel cross-sections each being defined by seventeen points. For any cross-section the value of z is constant. On a cross-section boundary x is the independent variable. When projected on the xz plane, these form a trapezoidal grid. The bases of the grid are the traces on the xz plane of the root and tip cross-sections of the airfoil. The sides are the xz projections of the leading and trailing edges.

The total x increment for each of the given cross-sections was divided by seventy-six and the Δz between each adjacent pair of cross-sections was divided by four, the result being 2233 intersections. The intermediate z values were calculated by hand. A program, using linear interpolation, was written to solve for the x values on cross-sections defined by the intermediate z values.

Another program was written to solve the value of y at each of the 2233 intersections for both the concave and convex surfaces of the blade. The method used was Newton's interpolation formula in terms of divided differences. At the conclusion of this program 2233 x values for points on the concave surface of the bucket form a data block near the end of drum storage. The corresponding values of y form another block which starts after the last x value and runs to the end of drum storage. The twenty-nine z values are held in magnetic core memory as program constants.

A third program was written which evaluates the normal to the concave surface at each of the above points with the exception of those on the edges of the surface. Each normal is the cross product of two vectors found by taking the first differences of x , y , and z between two points on either side of point P on the surface. One vector is in the cross-section plane. The other is in the longitudinal section plane. The program finds coordinates of P' , a point on the normal to the surface at P such that the distance from P to P' equals the radius of the ball end mill used in the machinery operation on the Numerically Controlled Milling Machine (NCMM). Included as constants in this program are six feed rates in terms of inches per minute. These were calculated by hand, it being decided from tool load conditions to change the feed rate at the end of the first, ninth, forty-seventh, and fifty-seventh passes of the tool. At the conclusion of this program there are in drum storage 2025 data blocks of four parameters each. These are feed rate in inches per minute and the x , y , and z coordinates of P' . These blocks are in proper sequence so that the tool center, when passing through consecutive points, will generate the convex surface of a die block that is in contact with the concave surface of the bucket during forging.

With the series of four parameter data blocks in drum storage, use was made of a program written by A. Siegel of the Digital Computer Laboratory Staff. The data blocks in storage are automatically translated into NCMM instructions by this program and the results are recorded on magnetic tape. After checking out the programs for interpolation and evaluation of points along the normals, a run was made in which Siegel's program was the final phase. The punched paper tape obtained from the magnetic tape output was given a trial run on the NCMM using a wooden mock-up of the die block. This NCMM program ran satisfactorily for seventy-three of the seventy-five tool passes programmed. Near the end of the seventy-fourth pass the program broke down. The cause was found to be in the computer program which evaluates points on the normals. There are several straight-forward methods of modifying the programs that prepare the data for Siegel's program so as to allow the NCMM program to be obtained in its entirety after a single computer run. Since time was not available to make a revision, it was expedient to recalculate the last two tool passes by resetting certain constants and counters in the program at fault. The results of this short run were spliced onto the NCMM tape at the beginning of the seventy-fourth pass. The corrected tape was rerun on the NCMM and the airfoil surface was cut on a steel block. The results obtained were, substantially, those anticipated.

This problem has been the subject of a bachelor's thesis entitled Numerical

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Control for Machining Warped Surfaces. The problem has been terminated and the thesis submitted to the Department of BUSINESS and Engineering Administration.

G. Bromfield
Business and Engineering
Administration

270 B. CRITICAL MASS CALCULATIONS FOR CYLINDRICAL GEOMETRY

The two-group, two-region method mentioned in the previous Summary Report has been used to calculate critical masses for uranium-aluminum-heavy-water cores surrounded by a heavy water reflector. On comparison with Snell's published data on this system, the calculated critical mass averaged about 30% lower than the experimental one. Most of this difference can be accounted for by the shortcomings of two-group theory. The neutrons slow down much faster in diffusion theory than is actually the case; therefore, a two-group model does not take into account all the fast leakage.

A parametric study of the effects of the fast diffusion coefficient and the age upon critical mass was made. As expected, critical mass was a strong function of the age, increasing with increasing age. The correct critical mass could not be obtained without increasing the age to a fantastic amount, however. Surprisingly, the fast diffusion coefficient had almost no effect. This is probably due to the strong thermalizing effect of heavy water: the fast flux drops almost to zero very quickly after leaving the core.

To obtain better agreement with experiment, a three-group approximation (mentioned in the last report) will be tried. Also, a numerical solution of the transport equation by the S_0 method will be attempted, with a large number of regions and groups. As cylindrical geometry presents difficult problems for this method, a solution will be tested first in spherical geometry, and then extended to cylindrical cases.

The two-group, two-region program is now being modified to obtain flux plots. From these, by numerical integration and perturbation theory, lifetimes and void coefficients will be calculated.

J. R. Powell
Chemical Engineering

271 B. EVALUATION OF A BEAM SPLITTING TECHNIQUE

This problem is concerned with a statistical estimation of target position in a radar system when the operating conditions are such that the echoes received from the target are corrupted by random noise and microwave interference. A brief description of the method is given in the previous Summary Report and in the S. M. thesis report entitled "Maximum Likelihood Estimation of Target Position in a Radar System With Gaussian Noise Distribution" submitted to the Department of Electrical Engineering in August, 1955, by Peter F. Engel.

The quantitative results of interest were the means and variances of the frequency distributions of the estimated positions, and the variation of these quantities with the radar system parameters. The means of the frequency distributions were biased away from the true target position by approximately two percent, or less, of the radar antenna's beam width, and the distributions had dispersions about the mean position of approximately seven percent of the antenna's beam width. The effect of doubling the antenna's angular velocity, thereby halving the sample size (or the number of received echo pulses), was to increase the azimuth dispersion by approximately twenty-five percent. Additional results of the computations are presented in the above-mentioned thesis report, and the problem has been terminated.

P. F. Engel
Electrical Engineering

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272 L. GENERAL RAYDIST SOLUTION

A program which derives the coefficients of an eighth degree polynomial and then proceeds to find a real root of the polynomial has been written. The program has proved to be quite contumacious and is still at the troubleshooting stage.

M. Rotenberg
Digital Computer Laboratory

273 N. ANALYSIS OF AIR SHOWER DATA

In Summary Report No. 42 there is a description of the main features of the data analysis program for the air shower experiment. That report describes how the program is divided into a data processing part, a timing analysis, and a pulse height analysis.

During the past three months the major errors in the program have been corrected and some testing has been done with an artificial air shower and a real one.

The data processing and timing analysis work satisfactorily. The main difficulties have been with the pulse height analysis. In the pulse height analysis we fit the function $f(\alpha, \beta, X, Y)$ to the data by the method of least squares. The variables are normalized so that they are dimensionless and are all of the same order of magnitude. We denote by g_1 the numerical value of an event recorded by the i th detector. For each g_1 there is an equation of the form

$$f_1(\alpha, \beta, X, Y) = g_1 + d_1, \quad i = 1, 2, \dots, N_{eq}$$

where

$$f_1(\alpha, \beta, X, Y) = f(\alpha, \beta, X, Y, x_1, y_1)$$

The numbers x_1, y_1 are constants associated with the i th detector; d_1 represents the unknown error in the measured quantity g_1 and also the error introduced by the poorness with which the empirical function f represents the true functional dependence of air showers. It is necessary to include d_1 in order to make the equations compatible for any given set of values of the variables α, β, X, Y . There are N_{eq} equations ($N_{eq} > 4$) and since there is a d_1 for each equation, the number of unknowns is $N_{eq} + 4$ so that there are infinitely many solutions. According to the method of least squares, the best solution is the one for which the following expression is a minimum:

$$\psi(\alpha, \beta, X, Y) = \sum_{i=1}^{N_{eq}} w_1 d_1^2 = \sum_{i=1}^{N_{eq}} w_1 (f_1 - g_1)^2$$

where w_1 is a weight which expresses the reliability of the observed value g_1 .

We represent the four variables by a vector $\vec{r} = (\alpha, \beta, X, Y)$ so that \vec{r} is a position vector in a four-dimensional cartesian coordinate system and ψ is a scalar function of \vec{r} . Let $\alpha_0, \beta_0, X_0, Y_0$ be initial guesses of the best values of α, β, X, Y (best in the sense described above). The present program minimizes ψ by an iterative process. If $\vec{r}_n = (\alpha_n, \beta_n, X_n, Y_n)$ is the position vector after the n th iteration, \vec{r}_{n+1} is given by

$$\vec{r}_{n+1} = \vec{r}_n - \lambda \frac{\text{grad } \psi(\vec{r}_n)}{|\text{grad } \psi(\vec{r}_n)|}, \quad n = 0, 1, 2, \dots$$

where λ is an arbitrary number which is chosen to make a reasonable change in \vec{r} per iteration. It is required that $\psi(\vec{r}_{n+1}) < \psi(\vec{r}_n)$ and that $\text{grad } \psi(\vec{r}_{n+1}) \cdot \text{grad } \psi(\vec{r}_n) > 0$. There are other conditions which must be satisfied but they are not important and will not be described here. The minimization routine used is LSR 141-201-271 (with slight modification).

The main difficulty with this iterative method is that it takes too much time to minimize ψ . At present it takes about three minutes for $N_{eq} = 20$. It is hoped that

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the time can be reduced to one minute. An effort will be made to speed up the evaluation of ψ and $\nabla^2 \psi$ by changing the empirical function f to a form more suitable for calculation on a digital computer. More drastic changes in the routine may be necessary and there is a possibility that the iterative method described here will be abandoned for some other procedure. We are planning to investigate another method described in reference 2.

References

1. DuMond, J. W. M., and Cohen, E. R., Least-Squares Adjustment of the Atomic Constants, 1952, Reviews of Modern Physics 25, No. 3, 691 (July, 1953).
2. Scarborough, J. B., Numerical Mathematical Analysis, second edition, The Johns Hopkins Press, 1950, p. 463.

G. W. Clark
F. Scherb
Physics Department

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

During the third quarter troubleshooting has continued on this problem. Production runs are expected to begin soon.

M. Karakashian
Joint Computing Group

277 C. HORIZONTAL STABILIZER MODES, SHAPES AND FREQUENCIES

A program developed under this problem number was used to determine the characteristic values $\{\lambda\}$ and eigenvectors $\{x\}$ for matrix equations of the type $A \cdot x = \lambda \cdot B \cdot x$.

L. Schmidt
Aeroelastic and Structures
Research Laboratory

278 N. ENERGY LEVELS OF DIATOMIC MOLECULES (LiH)

In the preceding Summary Report we described an investigation concerning the electronic energy of the lithium hydride molecule which is in progress. Extensive use is being made of Whirlwind facilities in evaluating the overlap, one-electron, and two-electron integrals for this molecule for a number of internuclear distances, and also for solving the resulting secular equations by diagonalization of the Hamiltonian and overlap matrices which are formed.

Results have been obtained for the complete configuration interaction problem at the observed internuclear distance in which we have used the Hartree-Fock 1s, 2s lithium wave functions, and a normalized 1s Slater Atomic Orbital for hydrogen. The result gave about one-half the observed binding energy, and was not appreciably different from the two-electron problem in which the 1s shell is kept filled. Therefore, we have extended the two-electron configuration interaction problem to several other internuclear distances, and it has been possible to construct a Morse curve quite accurately through the calculated points. This phase of the work will be extended to several additional internuclear distances.

The two-electron configuration interaction problem has been enlarged to include the possibility of one or both electrons occupying a lithium 2p orbital. Since the 2p energy levels lie near the 2s levels, it is expected that the value of the calculated binding energy should be somewhat improved by this treatment, although no results have been obtained at the moment.

A. M. Karo
Solid State and Molecular
Theory Group

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280 B. CORRELATION FUNCTION

As indicated in the initial report, this problem concerns the application of the theory of multiple time series prediction as developed by Norbert Wiener. From the practical standpoint, the most important concept of the theory is that an implicit factorization for single series permits a "factorization" for multiple series.

During this quarter, most of the time has been spent in perfecting transform programs and the program for single series factorization. Program work remaining includes multiple summation of multiple series, a recursion formula, and the prediction and error formulae.

It is hoped that research on this problem will continue in the next quarter.

F. Hanna
Meteorology

285 N. AUGMENTED PLANE WAVE METHOD AS APPLIED TO CHROMIUM CRYSTAL

Radial wave functions for a chromium crystal potential have been obtained for 13 " l " values and a grid of energies. From these, starting values for integration have been obtained at a distance from the origin. This step shortens the time required for obtaining U_l needed in the E vs. E_0 routine.

U_l

M. Saffren
Solid State and Molecular
Theory Group

288 N. ATOMIC WAVE FUNCTIONS

Calculations on the $3p$ states of C, Si, and Ge have been concluded. Similar calculations have been carried out, through the stage of evaluation of coefficients in the approximate linear expansion of self-consistent orbitals, for Mn and Mn^{2+} , both in $6S$ states.

R. K. Nesbet
Solid State and Molecular
Theory Group

291 B. DYNAMIC BUCKLING

This problem is concerned with the unstable motion of structural columns subjected to large, time-varying compressive loading. This motion may be in the elastic or plastic strain range of the column.

The elastic-plastic response of the column after the loads have been removed has been approximated by the use of a 12 degree-of-freedom lumped mass system. A second order of accuracy polynomial approximation integration procedure is used to integrate the equations. A program has been written and two successful runs have been made. Two additional runs are planned to complete this phase of the work.

The elastic response during the loading has been studied by expressing the deflection of the column by a combination of its normal modes. The Kutta-Gill procedure has been used to integrate the resulting equations. This motion has been calculated for four basically different variations of applied load versus time. One additional program may be run to secure additional data of this type.

The work described above has provided useful information about elastic-plastic vibrations and dynamic buckling response. It is anticipated that the next several days will complete this study.

R. E. Jones
Civil Engineering

296 C. SYSTEM ANALYSIS

This program has been collecting data for a classified project at the Instrumentation Laboratory. Numerically the problem involved the solution of seven simultaneous ordinary differential equations using the Gill routine.

This phase of the analysis has been successfully completed, but the system is still in the development stage. Therefore, we are keeping the problem number open anticipating that future computations will be necessary.

W. B. Kehl
Instrumentation Laboratory

297 B. DIFFUSION BOUNDARY LAYER

A suggested solution to the thermal problem at the boundaries of high speed surfaces is the injection of a coolant through a porous wall. As part of a doctoral thesis, the appropriate system of equations describing a compressible laminar boundary layer flow for a binary mixture have been developed to determine the effects of "foreign" coolants. Mass and thermal diffusion are included.

By means of Blasius and Dorodnitsyn type transformations, the system of equations reduces to three ordinary differential equations of the form (thermal diffusion neglected):

$$(\lambda r'')' + f r'' = 0$$

$$c_1'' + [f + (\alpha^{-1})'] \alpha c_1' = 0$$

$$\bar{T}'' + t_1 \bar{T}' + t_0 \bar{T} = t_m$$

which describe continuity of momentum, mass, and energy. f , c_1 , and \bar{T} represent velocity, fractional concentration by weight, and temperature, while λ relates the products of density and viscosity for the mixtures and external stream fluid. The remaining parameters are functions of Prandtl, Schmidt, and Mach numbers, as well as f , c_1 , the molecular weight ratio, and relative thermal capacities. Boundary conditions prescribe external stream conditions far from the surface, vanishing velocity at the surface, an injection rate, and, coupled with the latter, a concentration gradient such that no net flow of external fluid enters the surface.

Several approximate treatments of the equations are possible. When the Schmidt number is identically unity, the concentration is linearly related to the velocity. In addition, when temperature effects upon the relative magnitudes of the thermodynamic transport coefficients are negligible, the momentum and mass continuity relations are independent of the energy equation. Lastly, with an appropriate constant introduced into the original transformation, one may assume λ to be characterized by its surface value and thus employ the profuse prior information regarding the Blasius equation.

With the aid of Whirlwind, several of the mentioned simplifications are being evaluated using a Helium-Air mixture. Two point boundary conditions were replaced with initial estimates at the surface modified successively so as to yield an array of influence coefficients deduced from asymptotic results at infinity. (Infinity was essentially a value of 6.0 for the independent variable for asymptotic constancy to 5 significant figures.) The Gill-Kutta numerical integration procedure was employed. Programming included repeated integration cycles using the more exact boundary conditions resulting from the influence coefficient system until end conditions were satisfied to 5 significant figures. Generally, convergence to the proper values occurred within four cycles. In some cases, the tabulated Blasius function, f , and its derivatives were used in conjunction with a Taylor Series to yield the necessary intermediate values for the Gill-Kutta routine.

The results indicate appreciable reductions in the recovery (thermal equilibrium) temperature for a flat plate at relatively low injection rates. Due to the presence of the \bar{T} term in the energy equation, the recovery factor varies with Mach number. As a

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result, for certain injection rates and Mach numbers zero recovery factors are found. In all cases approximations to the exact equation yield conservative values. This is a consequence of the importance of the relative molecular weights for the components. Contemplated work is concerned with further examination of thermal diffusion effects as well as the limits for injection rates.

J. R. Baron
Naval Supersonic Laboratory

298 A. THE ELECTRONIC ENERGY OF THE HELIUM MOLECULAR ION

The potential interaction between a normal helium atom and a singly charged positive helium ion is of considerable interest in connection with the understanding of the collision processes occurring in gaseous helium. This interaction has been considered by Pauling (1933) and by Weinbaum (1935) who both used for the electronic wave functions of the Σ_g^+ and Σ_g^- states of He_2^+ the symmetrized forms

$$\Psi = \sum_{\lambda, \mu, \nu} [u(r_{A1}|Z) \phi(r_{B2}, r_{B3}) \mp u(r_{B1}|Z) \phi(r_{A2}, r_{A3})] X^{-\lambda, \mu, \nu} \quad (1)$$

where X^- is a doublet spin function given by

$$X^-(1, 2, 3) = \frac{1}{\sqrt{2}} (\alpha_1 \beta_2 - \alpha_2 \beta_1) \alpha_3 \quad (2)$$

and

$$u(r|Z) = \frac{1}{\sqrt{2\pi}} e^{-Zr} \quad (3)$$

$$\phi(r_1, r_2) = u(r_1|Z^1) u(r_2|Z^1) \quad (4)$$

the suffixes A and B referring to the two helium nuclei and 1, 2, 3, to the three electrons of the system.

Pauling took $Z = Z^1$ and determined the electronic binding energy by the Ritz variational method, while Weinbaum carried the calculations one stage further by varying the two exponential parameters independently. In the limit of large internuclear separation R it is found that $Z = 2$ and $Z^1 = 1.6875$ which corresponds to vanishing interaction between the He^+ ion and the He atom. In the case of the Σ_g^+ ground state of the helium molecular ion Weinbaum found that at the equilibrium position the exponential parameters had the values $Z = 2.029$ and $Z^1 = 1.734$, which are not very different from those obtained in the limit of large R , and consequently, that the improvement in the total electronic energy brought about by their variation was only slight.

Weinbaum's calculations correspond to using (4) as the unperturbed helium wave function for large internuclear separation. In the present work (4) has been replaced by the expression

$$\phi(r_1, r_2) = u(r_1|\alpha) u(r_2|\beta) + u(r_2|\alpha) u(r_1|\beta) \quad (5)$$

where the parameters α and β have been fixed at the values 2.19 and 1.18 respectively, corresponding to infinite separation between the helium atom and ion. This form for ϕ gives a rather better binding energy for the helium atom than does expression (4) used by Weinbaum. As before, the total electronic energy for the molecular ion can be determined by the application of the Ritz variational principle. The calculation involves the evaluation of one-electron, coulomb, hybrid and exchange molecular two-centre integrals for a wide range of internuclear distances. These were performed by the Whirlwind electronic computing machine using programs devised by Messrs. Corbatd, Dalgarno, and Merryman. The results of the calculation have not yet been fully analyzed, but will be available shortly.

In conclusion, it is a pleasure to express my thanks to Professor Morse,

Professor Slater, and Mr. Corbató for their assistance and interest in this work.

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B. L. Moiseiwitsch
Solid State and Molecular
Theory Group

299 C. HEAT TRANSFER IN TURBULENT FLOW

The physical situation analysed was that of a fluid flowing in well-developed turbulent flow in a smooth cylindrical pipe. The fluid initially at a uniform temperature T_1 enters a heated section having a constant wall temperature T_w greater than T_1 . It was desired to determine a relation between the heat transfer coefficient at any distance downstream and the physical and dynamic properties of the flowing fluid as characterized by the Prandtl and Reynolds numbers.

In order to generalize the solution, the following reduced variables are defined:

fraction of possible temperature change

$$\theta = \frac{T - T_1}{T_w - T_1} \quad (1)$$

reduced radius

$$y = r/R \quad (2)$$

and number of diameters downstream

$$x = z/D \quad (3)$$

The heat transfer coefficients are given in a generalized form in terms of Nusselt Numbers by the following expressions:

$$Nu = \frac{(Re)(Pr)}{4(1-\theta_0)} \cdot \frac{d\theta_0}{dx} \quad (4)$$

and the log mean Nusselt Number

$$Nu_M = \frac{-(Re)(Pr)}{4x\theta_0} - \ln(1-\theta_0) \quad (5)$$

θ_0 is the mixing cup mean θ at distance x given by

$$\theta_0 = \frac{\int_0^1 y u \theta dy}{\int_0^1 y u dy} \quad (6)$$

where u is the velocity at a reduced radius y . The fractional temperature change at any position is given by the partial differential equation

$$\frac{\partial \theta}{\partial x} = \frac{4B}{W} \left[\frac{\partial^2 \theta}{\partial y^2} + \left(\frac{1}{y} + \frac{d \ln B}{dy} \right) \frac{\partial \theta}{\partial y} \right] \quad (7)$$

with the boundary conditions

$$0 < y < 1.0 \quad x=0 \quad \theta=0 \quad (8)$$

$$y=0 \quad x>0 \quad \frac{\partial \theta}{\partial y} = 0 \quad (9)$$

$$y=1.0 \quad x>0 \quad \theta=1.0 \quad (10)$$

$$0 < y < 1.0 \quad x=\infty \quad \theta=1.0 \quad (11)$$

B and W are functions of y only, as given by the following:

$$W = (Re)(Pr) \sqrt{r/2} u^+ \quad (12)$$

$$B = 1 + \left(\frac{E}{\epsilon} \right) (Pr) \left[\frac{y}{du^+/dy^+} - 1 \right] \quad (13)$$

in which u^+ is a function of y^+ , a function of y

$$y^+ = (1-y) \left(\frac{Re}{2} \right) \sqrt{r/2} \quad (14)$$

The friction factor, f , is a function of Reynolds number and may be approximated by

$$\frac{f}{2} = 0.023(Re)^{-0.2} \quad (15)$$

The ratio of the eddy conductivity to the eddy viscosity, E/ϵ , was assumed to be unity.

The u^+ , y^+ relation used was as follows:

$$y^+ < 21.995 \quad u^+ = 13.5645 \tanh \left(\frac{y^+}{13.5645} \right) \quad (16)$$

$$y^+ \geq 21.995 \quad u^+ = 5.5 + 2.5 \ln y^+ - \frac{15}{y^+} \quad (17)$$

The constants were evaluated such that the function and its first derivative are matched at a y^+ of 21.995.

Solution of (7) was accomplished by means of a first order non-iterative finite difference method.

A variable spacing across the radius was employed for two reasons. One, the coefficients of the partial differential equation (7) approach infinity at the two boundary conditions, $y = 0$, and $y = 1.0$. Two, the so-called laminar layer at the wall is very small, especially with high Reynolds numbers, and therefore small increments are necessary if the effect of the laminar layer is to be included. If a stable solution is to be insured, very small x increments are also required, of the order of Δy squared or less.

In spite of the use of a variable y and x spacing, the number of repetitions required to obtain a solution is excessive. Ten thousand repetitions of the calculations in the region of the smallest x increment are required to calculate one diameter downstream. This calculation would take about 15 hours on the computer. If a steady state Nu is to be determined, approximately 70 to 100 diameters distance down-stream must be calculated.

As a test of the program, two very short runs (compared to the time required for

WHIRLWIND CODING AND APPLICATIONS

a complete solution) were made. One with the starting conditions specified of $\theta = 0$; and another in which a temperature distribution was assumed similar to a condition some three-quarters of the way through the calculation.

The program was successful. The results obtained were, of course, of little value. A complete description of the work in this problem will be presented in a Master's thesis in the Department of Chemical Engineering.

A. Turano
Chemical Engineering

300 L. TROPOSPHERIC PROPAGATION

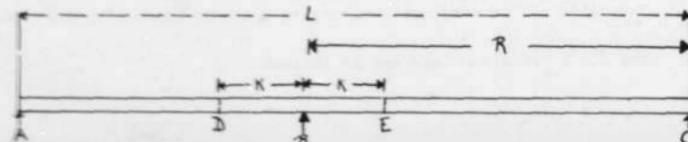
A tape was cut for the correlation of radio signal strength versus layers in radio refractive index. A pilot program was completed, and further use will be made of the tape in the future for the analysis of other data.

Values of a Fresnel integral have been computed, using a convergent power series with a complex argument. A number of satisfactory values have been obtained.

H.B. Dwight
Lincoln Laboratory

302 B. PARTIALLY CONTINUOUS WOODEN BEAMS

For certain applications in the Department of Building Construction, Mr. M. Barkan desired to find the properties of a wooden beam made up of two beams supported at the ends A and C and at the center of overlays B. The two beams are connected at D and E. The overall length from A to C is L. The other dimensions are fractions of L.



R is the distance from B to the nearer end C, which varies from .25 to .50 in steps of .05. K is the distance from B to the end of a component beam at D or E, which is to vary from .07 to .17 in steps of .01. W is the maximum deflection of the beam between A and B, which, it can be shown, is the maximum for the system. A uniform load W is assumed.

For each of these 66 cases, the forces acting at D and E, the bending moments, the shears and Y are to be found in terms of W, in which they are linear.

This leads to ten rational expressions in K and R of at most the eighth degree. The expression for Y is the maximum of a fifth degree polynomial in the distance from A, whose coefficients depend on previously computed quantities.

As the quantities that are used and those required have magnitude less than one, and as the accuracy required is within the four decimal digit range of the Whirlwind computer, this problem was solved without recourse to the interpreted CS computer. The primary reason this problem was presented to this Laboratory was to save time. A complete, accurate table of about 750 numbers was returned to Mr. Barkan about a week after he brought in his data and formula. It would have taken him about a month using a desk calculator.

M. Weinstein
Digital Computer Laboratory

WHIRLWIND CODING AND APPLICATIONS

303 B. PREDICTION OF CHROMATOGRAPHIC SEPARATIONS

Very little information is available for quantitative prediction of chromatographic separation by ion exchange. Hawthorn performed experimental work for the reversible, non-equilibrium case, where previous treatment is especially scanty. In addition to experimental work, Hawthorn developed a series of differential equations which describe the performance of an ion exchange column effecting a chromatographic separation of two cations. Attempts to obtain solutions to these equations were unsuccessful, but a method of numerical solution was presented.

As an extension of Hawthorn's work, this thesis proposes the following objectives:

1. Solution of the equations derived by Hawthorn through the use of the proposed numerical method and Whirlwind I.
2. Comparison of these solutions, which have a theoretical basis, with the experimental data.
3. Preparation of tables and graphs predicting elutriation curves for chromatographic separations for various parameters, if objective number 2 shows good agreement.

Re-examination of the basis for derivation of the differential equations, if objective number 2 shows poor agreement.

In order to achieve the above objectives, a program of instruction will be written for Whirlwind I. The first attempts will be kept as simple as possible, keeping close control on the adjustment of increment size, etc. Due to the complexity of the equations, the numerical method used will be the simple Euler method where it is assumed that

$$\frac{dy}{dy} \text{ or } \frac{du}{dx}$$

is constant over the respective increment. Convergence and stability of the solution will be checked by varying the increment size. If the calculated values show good agreement with the nine sets of experimental data reported by Hawthorn, the Whirlwind program will be refined, if necessary, and "production" runs will be performed for preparation of design tables and graphs.

The first two objectives listed above have been achieved. Solutions to the differential equations were found for two sets of parameters. Comparisons of these calculated results with experimental data give support to the validity of the assumptions used in the equation derivations.

The following tapes have been left on file at the Digital Computer Laboratory:

- | | |
|----------------|--------------------------------|
| fc 303-232-100 | } Convergence test |
| fc 303-232-20 | |
| fc 303-232-606 | } Elutriation curve prediction |
| fc 303-232-86 | |

A complete description of the procedures used and the results obtained is given in the M. S. Thesis, "Prediction of Chromatographic Separations by Ion Exchange Using Whirlwind I" submitted to the Chemical Engineering Department in August, 1955, by J. L. Fischer.

J. L. Fischer
Chemical Engineering

304 A. CALCULATIONS IN THE THEORY OF ATOMIC HYPERFINE STRUCTURE

Measurements of atomic hyperfine structure (hfs) contain some of the best information about the stationary electric and magnetic properties of atomic nuclei. In order to deduce accurate values for these nuclear properties (called nuclear moments), one must have an accurate evaluation of certain integrals over the electronic wavefunctions of the atom, (Ref. 1). These integrals have been evaluated previously (Ref. 2) by comparison with other atomic properties (the fine structure) using approximate but analytical wavefunctions which neglect the screening of the nuclear electrostatic potential. We decided to carry out a program of numerical computation of the wavefunctions and integrals, using a more realistic model for the atom. Since we require considerable accuracy in our results and expect to do the calculations for several atoms, this undertaking appeared feasible only with the use of a high-speed computer.

The equations to be solved are:

$$\left(\frac{d}{dx} - \frac{K}{x}\right) f = \left[1 - \frac{\alpha^2}{4} (\epsilon - 2V)\right] g$$

$$\left(\frac{d}{dx} + \frac{K}{x}\right) g = [\epsilon - 2V] f$$

where K, α are constants; $f(x), g(x)$ are the eigenfunctions; ϵ is the eigenvalue; and $V(x)$ is the potential seen by one electron in the atom. For this potential we use (Ref. 3):

$$V(x) = \frac{1}{x} \left[\frac{Z-1}{(1+\beta x)^2} + 1 \right]$$

where Z is the atomic nucleus and β is a parameter which will be adjusted to give the "best" results. The variable x may range from 0 to ∞ , but for physical and computational reasons, we have confined the study to $.0001 \leq x \leq 12$. This region is divided into 484 intervals, with spacings varying from 0.000005 to 0.1. Numerical integrations of the equations are done with the fourth-order Kutta-Gill subroutine. The ratio f/g at $x = .0001$ is determined from the boundary conditions that f, g be finite for $x \rightarrow 0$.

The main problem is to find the value of the eigenvalue ϵ which makes f and g go to zero as x goes to ∞ . Our method of finding ϵ is patterned after that used by Combelic, (Ref. 4). With some guessed value of ϵ the equations are integrated out to some large value of x, x_0 (we use $x_0 = 12$). For $x > x_0$ we set $V = 0$ and the solutions f, g for this outer region are then known in terms of spherical Hankel functions. The inner and outer solutions are then joined at x_0 :

$$g(x_0), f(x_0) \sim C_1 h^{(1)}(ikx_0) + C_2 h^{(2)}(ikx_0)$$

where the order of the Hankel functions depends on the constant K and $k \approx \sqrt{\epsilon}$. Since the asymptotic value of these functions is:

$$h^{(1)}(ikx) \rightarrow e^{-kh}$$

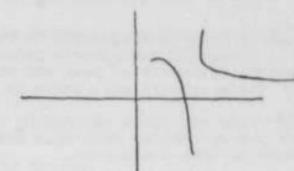
$$h^{(2)}(ikx) \rightarrow e^{kh}$$

the eigenvalue condition is $C_2 = 0$. Thus a linear combination of $f(x_0)$ and $g(x_0)$ multiplied by simple polynomials in $(kx_0)^{-1}$ gives the quantity $C_1 e^{kx_0}$ which we take as our error function $\mathcal{E}(\epsilon)$. Then repeating the integration of the differential equations with new values of ϵ we find the eigenvalue ϵ_0 for which $\mathcal{E}(\epsilon_0) = 0$. With a fairly good initial guess for ϵ we can find ϵ_0 to about one part in 10^5 or better in 3 to 5 iterations.

It is probably worth noting that there are several ways in which one should not go about searching for the eigenvalue ϵ_0 . If one defines $\mathcal{E}(\epsilon)$ from some such "normalized" form as

$$f(x_0)/g(x_0), f'(x_0)/f(x_0), C_2/C_1, \text{ etc.},$$

the denominator of each of the quotients has a zero very close to where \mathcal{E} passes through zero, and it is very difficult to find the zero of a function which looks like the drawing on the next page.



Here the width of the interesting region is extremely small ($\sim 10^{-7}$ in our problems).

An alternative procedure used was to put in the desired (experimentally measured) value of ϵ and find the value of β (the potential parameter) that satisfies the eigenvalue criterion. When the eigenvalue is found, the several integrals of interest,

$$\int_0^{\infty} (r^2 + g^2) dx, \int_0^{\infty} (r^2 + g^2) x^{-3} dx, \int_0^{\infty} f g x^{-2} dx, \int_0^{\infty} f g x^{-4} dx,$$

are computed with the eigenfunctions using fourth-order integration.

So far, these calculations have been carried out for the p-doublet ground states of eight different atoms spanning the entire periodic table. The results are in some cases significantly different from the results of the earlier work. There are still a few more calculations to be carried out. A careful analysis of results in comparison with experimental data is expected to yield the values of the nuclear moments accurate to within a very small per cent.

References

1. C. Schwartz, Phys. Rev. 97, 380 (1955).
2. H. B. G. Casimir, *On the Interactions Between Atomic Nuclei and Electrons*, Teler's Tweede Genootschap, Haarlem, 1936.
3. T. Tietz, J. Chem. Phys. 22, 2094 (1954).
4. D. Combelic, Project Whirlwind Summary Report No. 30, Problem No. 60, page 17 (1952).

Charles Schwartz
Research Laboratory of Electronics

305 A. COURSE 6.25, MACHINE-AIDED ANALYSIS

Fifteen students in the summer section of 6.25, a course in machine-aided analysis in the department of Electrical Engineering, used TAC to solve a homework problem. The problem, involving the generation of a sine function and the solution of a differential equation, was designed to illustrate the use of an actual computer for solving numerical problems. As is the usual case when students are first introduced to a digital computer, about 60% of the students had programs work correctly the first time.

W. J. Eccles
Electrical Engineering

306 D. SPECTRAL ANALYSIS OF ATMOSPHERIC DATA

Recent theoretical, observational and experimental studies (conducted at M.I.T. and other institutions) have demonstrated that the wave-like disturbances (eddies) in the atmosphere are of primary importance in generating and maintaining the mean global field of motion. To a large degree, the form of these eddies characterizes the state of the general circulation. Little quantitative information has been obtained, however, as to the exact

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scales of these atmospheric disturbances and the contribution which the different scales of disturbances make to certain dynamically significant processes such as the transport of heat and momentum.

Accordingly, it is the purpose of this investigation to obtain long series of latitudinal space spectra for a number of important atmospheric properties (kinetic energy, temperature, water vapor, vertical velocity, transport of heat and momentum) as a function of latitude, pressure-height, and time. These spectra will serve as the basis for:

1. Providing a picture of the time and space variations of the spectral distributions of significant atmospheric parameters, as well as a measure of the relative importance of the various scales of eddies in that atmosphere.
2. Testing the results of certain theoretical models of the atmospheric flow, regarding the stability properties of disturbances.
3. Relating changes in the kinetic energy spectral distribution to other important parameters.
4. Studying the dynamic interactions among disturbances of different scales and the mean flow.

In more concrete terms, it is proposed to obtain the spectra for the 1000, 700, 500, 300, and 200 mb pressure surfaces at latitudes 30°, 45°, and 60°N.

The spectra will be based on data obtained at 72 points (every 5 degrees of longitude) around a latitude circle and will be computed for wave numbers 1 through 15 by means of the standard methods of harmonic analysis. In general, the complex spectral function for any property, q , is given by

$$F(n) = p_1(n) + i p_2(n)$$

where

$$p_1(n) = \frac{1}{72} \sum_{\lambda=1}^{72} q(\lambda) \cos n\lambda$$

$$p_2(n) = \frac{1}{72} \sum_{\lambda=1}^{72} q(\lambda) \sin n\lambda \quad (\lambda = 0^\circ, 5^\circ, 10^\circ, \dots, 355^\circ)$$

Here λ represents longitude and n is the wave number.

By suitably combining the Fourier coefficients for the heights of the pressure surfaces, temperature, the zonal wind, water vapor and vertical motion it is possible to obtain all of the desired transport spectra and the kinetic energy spectra. For example, the spectral function, $T(n)$, for the meridional transport of sensible heat for a given latitude ψ , pressure p , and time t , is given by

$$T_{\psi,p,t}(n) = n [b_2(n)a_1(n) - b_1(n)a_2(n)] \psi, p, t$$

where a_1 and a_2 are the real and imaginary parts, respectively, of the pressure-height spectrum, and b_1 and b_2 are the components of the temperature spectra.

The spectral function for the geostrophic kinetic energy of the north-south flow is given simply by

$$K_{\psi,p,t}(n) = n^2 [a_1(n)^2 + a_2(n)^2]$$

It is anticipated that complete hemispheric data for the month of January, 1949, as well as a much longer series of height data for the 500 mb level alone, will be processed.

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Extensive computations of the type outlined above have become feasible only with the advent of high-speed machines such as WWI.

The program is currently in the process of being checked.

B. Saltzman
F. Ward
Meteorology

307 C. SUPERSONIC NOZZLE DESIGN

The Friedrichs method employed at the Naval Supersonic Laboratory for deducing supersonic nozzle contours has been programmed for Whirlwind. On the basis of an assumed velocity distribution (nozzle generating function) along a reference axis, there follow expressions for the physical coordinates and flow properties along streamlines for a perfect gas expanding from subsonic to supersonic speed. It is required that the exhaust flow be uniform and parallel for model test purposes. Each design (exit) Mach number therefore necessitates a numerical integration process to establish the flow properties along a (design) characteristic in the supersonic field. Downstream of the latter characteristic line, streamlines are determined on a mass continuity basis such that a Prandtl-Meyer flow region precedes the final uniform flow field.

The Gill-Kutta procedure was employed for the numerical integration portion of the program. Application of the Newton-Raphson method was made to find certain Mach number distributions at equal coordinate intervals.

The program has been initially successful and is currently being checked in detail against earlier computations. It is intended to make use of the program for future nozzle requirements at the Naval Supersonic Laboratory.

J. R. Baron
Naval Supersonic Laboratory

308 A. FREQUENCY ANALYSIS OF APERIODIC FUNCTIONS

This problem is a continuation of problem 195C. We now plan to generate cosine functions of different frequencies and cross correlate each function with the intestinal motility data. We then will calculate the root mean square values of these cross correlation functions.

J. Roseman
Digital Computer Laboratory

309 B.N. PURE AND IMPURE KCl CRYSTAL

A theoretical study is to be made of the electronic structure of an alkali halide crystal. The free-ion, Hartree-Fock wavefunctions will serve as a starting point of the study. Since an alkali halide in its ground state is a closed shell system, the ground state wavefunction may be approximated by a single Slater determinant of the normally occupied, free-ion functions. Due to the small overlap of these functions in the crystal, the approximation is fairly good. If the determinant is made up of linear combinations of these free-ion functions, the crystal energy is of course unchanged. For the perfect crystal it is proposed to determine one-electron wavefunctions as those particular orthonormal linear combinations of the free-ion functions which satisfy the Bloch condition and which satisfy the Hartree-Fock equations. From this the Hartree-Fock energy band structure of the crystal will be obtained and can be compared to recent X-ray studies.

It is further proposed to study the V-center as a particular example of the impure or almost perfect crystal. The V-center in an alkali halide crystal is a positive ion vacancy with an associated, bound hole (an electron vacancy in an otherwise closed shell structure). The many-electron wavefunction can again be approximated by a single determinant which is made up of linear combinations of free-ion functions. Using an argument due to Koopmans, however, this wavefunction is completely determined when the coefficients of only the missing electron are known. Thus the crystal energy for various

states of excitation of the hole can be determined by solution of a finite secular equation. Because of the localized nature of the impurity, the secular equation need only involve free-ion functions on sites near the impurity center. This calculation does not depend on any preliminary, perfect crystal calculation. It is thus proposed to determine transition energies for the bound hole and compare the results to recent experimental observations.

In both the pure and impure crystal problems described above, we must solve a set of simultaneous eigenvalue equations of the following form:

$$\sum_m (H_{nm} - \epsilon \Delta_{nm}) a_m = 0,$$

where the a_m 's are the coefficients of free-ion functions or linear, symmetry combinations of free-ion functions, and H_{nm} and Δ_{nm} are respectively energy and overlap integrals. The integrals are closely related in the two problems of this paper; hence the problems are being performed together.

Many of the integrals involved are between functions on different centers in the lattice. These integrals are to be evaluated by the expansion method of Barnett and Coulson as adapted for Whirlwind use by F. J. Corbató of this group. In this method, an integral between wavefunctions on different centers is calculated by choosing one of the centers and expanding all of the displaced functions in a series of radial functions (called $Q(r)$ by Corbató) times spherical harmonics about that center. For two-electron integrals $1/r_{12}$ is also expanded in spherical harmonics about the common center. The original integral then becomes a finite or infinite sum of integrals, each of which can be calculated easily.

The order of calculation is as follows. The Hartree-Fock radial functions for Cl^- and K^- are fitted with sums of exponentials times powers of r . The resultant analytic functions are expanded about another center using Corbató's Alpha-Generation Program (named for the coefficients $\alpha(r)$). Certain linear combinations of the alphas are performed by my own Mode Addition Program. Finally the basic integrals are calculated by Whirlwind using Corbató's Integrator Program. The basic integrals are then combined by hand to form the H_{nm} and Δ_{nm} mentioned above. Finally the secular equations for the a_m 's and the ϵ 's are solved on Whirlwind using routines developed by Meckler and Corbató. All of the programs mentioned have now been tested and have been found satisfactory. It is therefore expected that by the end of the next quarter most of the production runs will have been completed.

L. F. Howland
Solid State and Molecular
Theory Group

310 C. TRAJECTORY CALCULATIONS FOR A ROCKET DURING POWERED FLIGHT

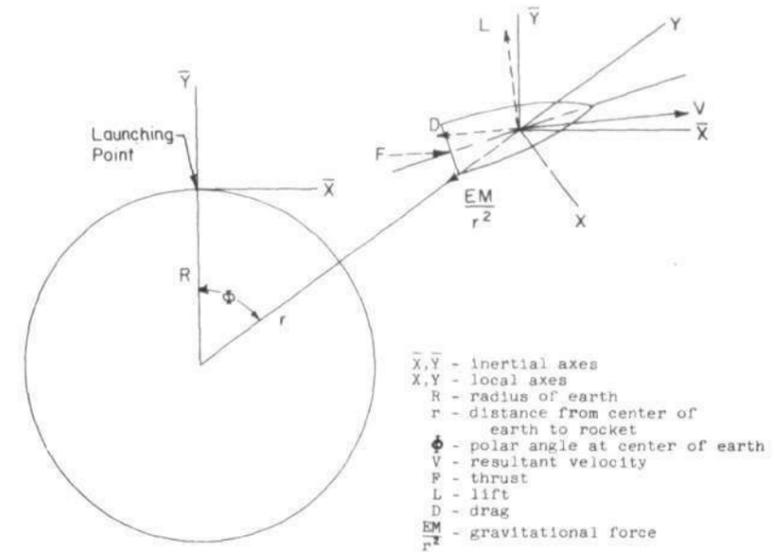
A rocket obeys Kepler's Laws when it is in free flight, since no exterior forces are applied; however, when the rocket's engines are providing thrust Kepler's Laws no longer apply. Consequently, in order to find the optimum powered-flight trajectory, i.e., the trajectory which uses the least amount of fuel, it is necessary to do a trial and error trajectory study. A further complication is the effect of the atmosphere on the rocket, namely the forces of drag and lift. The equations of motion of a rocket during powered flight, taking into consideration all the forces that have been mentioned, are then

$$\frac{d^2 r}{dt^2} - r \left(\frac{d\Phi}{dt} \right)^2 = \frac{F}{M} \sin(\theta - \delta) - \frac{D}{M} \sin \gamma + \frac{L}{M} \cos \gamma - \frac{E}{r^2}$$

$$r \frac{d^2 \Phi}{dt^2} + 2 \frac{dr}{dt} \frac{d\Phi}{dt} = \frac{F}{M} \cos(\theta - \delta) - \frac{D}{M} \cos \gamma - \frac{L}{M} \sin \gamma$$

where the equations are written with reference to axes aligned with the local vertical. (Figure 1 defines the nomenclature used in the above equations.)

DEFINITION OF QUANTITIES USED IN EQUATIONS OF MOTION



- α - angle of attack
- δ - rocket engine deflection
- θ - pitch angle } with respect to
- γ - flight path angle } local horizontal
- θ - pitch angle } with respect to
- $\bar{\gamma}$ - flight path angle } inertial horizontal

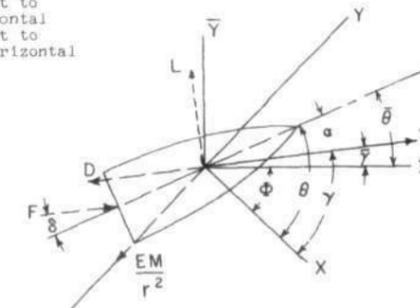


FIGURE 1

For the purposes of this investigation the equations of motion were written in the following non-dimensional form

$$\frac{d^2 n_N}{d\tau^2} - n_N \left(\frac{d\bar{\theta}}{d\tau} \right)^2 = \bar{E} \left\{ \eta_F \frac{F_N}{M_N} \sin(\theta - \delta) - \eta_D \sin \gamma + \eta_L \cos \gamma \right\} \left(\frac{\partial_z}{\partial R} \right) - \frac{\bar{E}}{n_N}$$

$$n_N \frac{d^2 \bar{\theta}}{d\tau^2} + 2 \frac{dn_N}{d\tau} \frac{d\bar{\theta}}{d\tau} = \bar{E} \left\{ \eta_F \frac{F_N}{M_N} \cos(\theta - \delta) - \eta_D \cos \gamma - \eta_L \sin \gamma \right\} \left(\frac{\partial_z}{\partial R} \right)$$

where

$$n_N = \frac{n}{R}$$

$$\bar{E} = \frac{E}{V_s^2 R} = 1$$

$$\eta_F = \frac{F_z}{W_z} = \frac{\bar{J}_z I_{sp}}{I_b}$$

$$F_N = \frac{F}{F_z} = \frac{C_1 \frac{F}{F_z} + C_2 \frac{P^*}{P_{sl}}}{C_1 \frac{P_0}{P_{sl}} + C_2 \frac{P_0^*}{P_{sl}}}$$

$$M_N = \frac{M}{M_z} = 1 - \frac{R \bar{J}_z}{V_s t_b} \int_{\tau_2}^{\tau_f} \dot{m}_N d\tau$$

$$\bar{J}_z = \frac{\dot{m}_z t_b}{M_z}$$

$$\dot{m}_N = \frac{\dot{m}}{\dot{m}_z} = \frac{\frac{\bar{P}_z}{P_{sl}} + \frac{P^*}{P_{sl}}}{\frac{P_0}{P_{sl}} + \frac{P_0^*}{P_{sl}}}$$

$$\eta_D = \frac{D}{W} = \frac{V_s^2}{2} \left(\frac{C_{Dz}}{\mu} \right) \left(\frac{P}{P_{sl}} \right) \frac{C_D}{M_N} \bar{V}^2$$

$$\eta_L = \frac{L}{W} = \frac{V_s^2}{2} \left(\frac{C_{Lz}}{\mu} \right) \left(\frac{P}{P_{sl}} \right) \frac{C_D}{M_N} \bar{V}^2$$

$$\bar{V} = \frac{V}{V_s} = \frac{dn_N}{d\tau} \sin \gamma + n_N \frac{d\bar{\theta}}{d\tau} \cos \gamma$$

$$I_{spz} = \frac{F_z}{\dot{m}_z g_s} = \frac{\eta_L \eta_F}{\eta_{\dot{m}}} \left[\frac{C_1 \frac{P_0}{P_{sl}} + C_2 \frac{P_0^*}{P_{sl}}}{C_3 C_4 \left(\frac{P_0}{P_{sl}} + \frac{P_0^*}{P_{sl}} \right)} \right]$$

$$\frac{A_z}{A_e} = \left(\frac{k+1}{2} \right)^{\frac{k-1}{k}} \left(\frac{P_0}{P_c} \right)^{\frac{k}{k-1}} \sqrt{\frac{k+1}{k-1} \left[1 - \left(\frac{P_0}{P_c} \right)^{\frac{k-1}{k}} \right]}$$

$$C_1 = \left\{ \sqrt{\frac{2k^2}{k-1} \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left[1 - \left(\frac{P_0}{P_c} \right)^{\frac{k-1}{k}} \right]} + \left(\frac{P_0}{P_c} \right) \left(\frac{A_e}{A_z} \right) \right\}$$

$$C_2 = \left\{ \sqrt{\frac{2k^2}{k-1} \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left[1 - \left(\frac{P_0}{P_c} \right)^{\frac{k-1}{k}} \right]} + \left(\frac{P_0}{P_c} - 1 \right) \left(\frac{A_e}{A_z} \right) \right\}$$

$$C_3 = \sqrt{k \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}}}$$

$$C_4 = \sqrt{\frac{g_s}{R T_c}}$$

$$\gamma = \tan^{-1} \frac{\frac{dn_N}{d\tau}}{n_N \frac{d\bar{\theta}}{d\tau}}$$

$$\tau = \frac{t V_s}{R}$$

$\Theta =$ forcing function

A typical trajectory is shown in Figure 2. In order to optimize the trajectory, various parameters must be varied, such as the length of time spent in vertical flight, the impulse angle-of-attack at tip-over, the length of time before staging, the length of time before burnout, and the pitch-program used. For any given set of parameters the

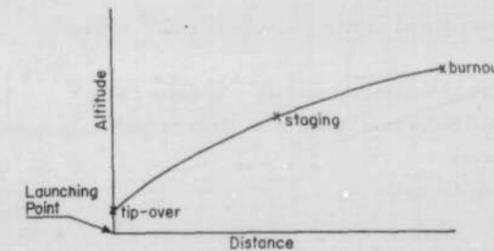


FIGURE 2

velocity, flight path angle, altitude, and distance from launching point at burnout must be those which will cause the following equation to become zero.

$$\delta = \frac{\bar{E}}{R_W (\bar{V} \cos \gamma)^2} \left[1 - \cos(\Phi_T - \Phi) \right] + \cos(\Phi_T - \Phi) - \tan \gamma \sin(\Phi_T - \Phi) - R_W$$

where Φ_T is the specified range.

The first routine written for CSII was one which evaluated

$$\frac{P_e}{P_c}, C_1, C_2, \text{ and } C_3$$

for various values of k and $\frac{A_e}{A_t}$. Since then all work has been concentrated on writing subroutines for the main program. Subroutines which have been written and checked are determination of pressure, density, and temperature at any arbitrary altitude from sea level to 128,900 meters; evaluation of C_D from mathematical representations of the curve of C_D versus Mach number at any arbitrary Mach number; and determination of the burnout point through use of the δ equation given above, including a sixth order interpolation routine for evaluating the various parameters at the burnout point.

During the next quarter further subroutines will be written and checked out, and the main program itself will be written. Trial runs will then be made and compared with check solutions, which have been computed on an IBM-CPC.

The program thus far has been written by Granger G. Sutton, Research Engineer under the supervision of John S. Prigge, Jr., Project Leader of DIC Project 7246, both of the Aerophysics Research Group, Department of Aeronautical Engineering. The work is sponsored by the U. S. Air Force under Contract No. AF 33(616)-2392 and will eventually be issued as a formal report.

Definition of Symbols

A	area
C_D	drag coefficient
C_L	lift coefficient
D	drag
E	earth's gravitational factor = 1.4086414×10^{16} ft ³ /sec ²
F	thrust
g_R	absolute gravity at earth's surface = 32.28512 ft/sec ²
g_s	gravitational conversion factor = 32.17405 ft/sec ²
Isp	specific thrust
k	ratio of specific heat
L	lift
\dot{m}	propellant mass flow
M	mass
n	load factor
p	pressure, absolute
\bar{p}	pressure, gage
r	distance from center of earth to rocket
R	radius of earth = 20.888104×10^6 ft.

R	gas constant
t_b	burning time
T	temperature, absolute
V	velocity
V_s	velocity of satellite at earth's surface = $\sqrt{g_R R} = 25.968730 \times 10^3$ ft/sec
W	weight

Greek Letters

γ	flight path angle
δ	rocket engine deflection
\bar{J}	pseudo propellant load factor
η	efficiency
η_λ	divergence loss of a nozzle
θ	pitch angle
μ	weight loading factor = $\frac{M_1 g_s}{A}$
ρ	density
τ	non-dimensional time
Φ	polar angle measured from center of earth

Superscripts

.	ambient value
-	non-dimensional (with exception of \bar{p})

Subscripts

c	chamber
e	exit
f	final value
F	thrust
\dot{m}	propellant mass flow
N	normalized with respect to initial value
P	propellant
s	satellite
SL	sea level value
t	throat

J. S. Prigge, Jr.
Aerophysics Research Group

WHIRLWIND CODING AND APPLICATIONS

311 N. SOLITARY WAVE GENERATING CAM

This is the first quarterly progress report on Problem 311 N. The problem consists in the solution to a series of algebraic equations which describe the loci of the tool centers for work to be executed by the numerically-controlled milling machine of the Servomechanisms Laboratory. The work for the milling machine is the cutting of stainless-steel cams to be used with the wave machine of the Hydrodynamics Laboratory, as part of the work carried out on the Solitary Wave Research Project, DIC 3-6664, conducted for the Office of Naval Research under Contract No. N5ori-07837.

The form of the cams is two half-length sine waves superimposed on a neutral circle of the cam. The ratio of the two wave lengths varies from 1:16 to 1:1 for a series of eight cams. The equations for the cam surfaces were modified to account for the center position of the milling machine tool during cutting.

The input to the milling machine is binary punched tape; therefore, a Whirlwind subroutine developed by John Runyon was used to convert the decimal results to the algebraic equations to binary punched tapes.

The programmers for this problem are Donald C. Taylor and John G. Housley of the Hydrodynamics Laboratory. Technical assistance in programming was given by Mr. A. Siegel of the Digital Computer Laboratory staff.

J. G. Housley
Hydrodynamics Laboratory

312 L. ERROR ANALYSIS

The errors in the knowledge of a set of six parameters descriptive of a system are to be determined from the errors in certain measurements on the system. These measurements are assumed to be corrupted by additive gaussian noise. A small error approximation is made so that errors in the parameters are linear in the measurement errors. The parameter errors are, therefore, also gaussian. Whirlwind I will compute the moment matrices of the errors in the parameters for various input conditions.

The problem can be stated mathematically as the evaluation of a 4×6 and a 6×6 matrix. The elements of these matrices are functions of six parameters and a variable of integration, whose values will be determined from the limits of integration to be described below. The functions require the evaluation of square roots, trigonometric and inverse trigonometric functions. The parameters will be given as input conditions and the results determined for various sets of these parameters. The two matrices are to be multiplied together to yield a third matrix, the elements of which will be multiplied together two at a time and each pair integrated. The limits of integration will be supplied and the results again determined for various sets of values. The integrals will form the elements of four 6×6 matrices which are to be added together with weighting factors which will also assume various values. The resulting 6×6 matrix is to be inverted and then premultiplied by a 2×6 matrix and postmultiplied by the transpose of this matrix. The elements of the 2×6 matrix will be functions of the six parameters mentioned above and will require evaluation of the same basic functions. The final 2×2 matrix is to be diagonalized. The inverted 6×6 matrix, the eigenvalues and one eigenvector of the 2×2 matrix are desired as final results. The various combinations of input values needed will require approximately 100 repetitions for the basic procedures described.

The program has already been tested and will be used in the near future.

I. I. Shapiro
Lincoln Laboratory

WHIRLWIND CODING AND APPLICATIONS

313 D. COURSE 6.601, NUMERICAL CONTROL OF MACHINE TOOLS

As part of Course 6.601, the students are required to produce, using manual computation, a program for the Numerically-Controlled Milling Machine (NCMM). Because of time limitations, they are not required to carry their computations to completion but are permitted to stop at an intermediate point at which the remaining calculations are obvious.

A Whirlwind I routine was prepared which completed the students' computations and punched the resulting NCMM control tape. This routine was used to process all the data provided by the students, and the tapes were then used on the NCMM. The routine operated correctly, and produced satisfactory NCMM tapes.

A tour of the WWI computer, during which was demonstrated the NCMM translation program developed under problem 250, was arranged as part of the course.

A. Siegel
Digital Computer Laboratory

314 C. FACTORING HIGH ORDER POLYNOMIALS

This problem concerns the analysis of the effects of aircraft flexure coupling with aircraft automatic control systems. The analysis results in two sets of six simultaneous differential equations of motion. Whirlwind was used to determine the roots of the resulting performance functions. Factorization of several polynomials of about the 10th degree was done using Hitchcock's method, for which programs were written by M. Jacobs of the Digital Computer Laboratory.

V. W. Howard
Aeroelastic and Structures
Research Laboratory

316 L. RADAR CORRELATION

A method is sought to correlate on a real time electronic computer the data that may be found directly by radar apparatus.

Some time was spent to determine the analytic solutions which would have the least inherent error and would allow high-speed computation.

To minimize error in a function of more than one variable, a linear programming routine is being developed. This routine has already been checked in part and is now being modified to take advantage of new instructions pertaining to access to the magnetic drum storage. By evaluating the exact expression at several points and then letting the coefficients in a simplified expression be variable, we should be able to find coefficients that minimize the maximum error.

M. Weinstein
Digital Computer Laboratory

WHIRLWIND CODING AND APPLICATIONS

NOTE:

Reports on the following problems, done by members of the Machine Methods of Computation group, may be found in Section 2.2 of Part I.

122 N.	COULOMB WAVE FUNCTIONS	A. Temkin Z. Fried A. Tubis
172 B.N.	ENERGY BANDS IN GRAPHITE	F. Corbató
217 N.	ATOMIC WAVE FUNCTIONS AND ENERGIES	A. Tubis
235 B.N.	EIGENVALUES IN A SPHEROIDAL WELL	J. Uretsky
242 N.	CALCULATION OF NUMBERS OF STRUCTURES OF RELATIONS ON FINITE SETS	D. McIlroy

APPENDIX

1. SYSTEMS ENGINEERING

Magnetic Drums

The interlace on the auxiliary section of the buffer drum has been changed to provide more rapid access to drum storage. The computer may now read or record blocks of information at the rate of one word every 32 microseconds. The former rate was one word every 64 microseconds.

The control systems for both drums have been modified to permit the selection of a new mode of operation. The programmer, by adding 1000 (octal) to the present drum orders, may select the drum as a consecutively addressed storage medium with no discontinuities at the end of each group. The Group Selection Register (GSR) has been made a counter which is added to by the end carry from the Storage Address Register (SAR). The SAR end carry to GSR is gated by digit 6 of the in-out switch.

Magnetic Tape

In several instances, valuable information recorded on magnetic tape has been destroyed by accidental recordings over this information. A system has been installed to allow the three printout units to be locked in the read mode by means of toggle switches located on their control panels. The computer may sense an intervention bit to determine whether these switches have been thrown or whether the units are ready to record.

Power Supplies

A spare filament alternator has been obtained and the installation work necessary for connecting it into the system is in progress. The control system will be such that the alternator may be used to replace either of the two alternators now in service by operating one or two toggle switches. A system for substituting a motor-generator set for one of the d-c supplies is being developed.

Polaroid Land Camera

A Crown-Graphic camera with a Polaroid Land-camera back has been mounted in the control room for photographing the indicator lights. The photographs may be used in place of manual recordings of the lights. This system provides a sure, fast, accurate means of gathering trouble-location information.

Computer Reliability 17 June 1955 to 22 September 1955

Total computer operating time	2017	hours
Total lost time	54.4	hours
Percentage operating time usable	97.4	percent
Average uninterrupted operating time between failures	14.2	hours
Failure incidents per 24-hour day	1.65	
Average lost time per incident	23.6	minutes
Average preventive maintenance time per day	1.5	hours

APPENDIX

2. VACUUM TUBES

Vacuum Tube Life

During the first three quarters of 1955, the Whirlwind computer operated for 1780, 1932, and 1880 hours, respectively. Vacuum tube life has been calculated for the six most numerous types in WWI, comprising approximately 80% of the total tube complement. A summary of this information is shown below:

Tube Type	Quantity now in Service	FAILURE RATE, PER CENT 1000 HOURS			
		1954 Average	First Quarter 1955	Second Quarter 1955	Third Quarter 1955
7AD7/SR1407/6145	4273	1.5	0.97	1.1	0.69
7AK7	3400	0.44	0.25	0.18	0.08
5965	887	0.32	0.38	0.52	0.60
6080/6080WA/6AS7G	712	1.1	0.48	2.0	3.5
6BL7GT	496	0.41	0.46	0.52	0.96

The number of 2D21 failures has been materially reduced as a result of circuit changes correcting excessively negative grid voltage during conduction (see Summary Report No. 40, Fourth Quarter, 1954).

The number of 5963 failures has been steadily decreasing. This is because most of the older tubes of the original complement have already failed due to cathode interface impedance and have been replaced; the present failures either went into service after the original equipment installation or are in circuits where operating margins are wider and hence more tolerable of tube deterioration.

The type 5965 continues to be quite stable, from a maintenance-of-characteristics point of view: practically all the failures in this type are due to high negative grid current, primarily leakage, with some grid emission beginning in the older tubes.

The relatively large fluctuations in the failure rate of 7AK7's are caused by statistical variations in the small number of failures per quarter. The failure rate for this type continues to be comfortably low.

The type 6BL7GT has now reached approximately 12,000 hours of operation. Although the failure rate has been relatively low, it has been increasing as a result of a small but increasing number of low-plate-current failures partially due to cathode interface impedance. The sharp increase in the failure rate during the third quarter of 1955 is a result of the routine retesting of a panel temporarily removed from WWI service and the subsequent failure, at test, of seven tubes for low plate current. The circuits in which these tubes operate (cathode follower being driven by a cathode follower) are such that a considerable decrease in zero-bias plate current can be tolerated before system failure begins. The extremely low zero-bias plate current cannot be completely ascribed to the magnitude of cathode interface impedance involved (100-200 ohms). Qualitative tests indicate a major decrease in cathode emission itself.

Some comment is in order regarding the high failure rate of the types 6080/6080WA. A considerable quantity of these tubes is used in series-tube-regulator panels where, prior to a recent modification, circuit conditions were such that the tubes were being operated considerably over plate dissipation rating. In the magnetic core memory system where operating conditions are much less severe, the failure rate of this type continues to be reasonably low.

APPENDIX

3. PUBLICATIONS

Project Whirlwind technical reports and memoranda are routinely distributed to only a restricted group known to have a particular interest in the Project and to ASTIA (Armed Services Technical Information Agency) Document Service Center, Knott Building, Dayton, Ohio. Requests for copies of individual reports should be made to ASTIA.

The following is a list of memoranda published by the Scientific and Engineering Computations Group during the past quarter.

No.				
DCL-81	Abstracts of memos on Automatic Coding Techniques Used on WWI	6-22-55	J. M. Frankovich	
DCL-82	A Proposal for a New Method of Selecting the WWI Drums for Block Transfers of Information	6-21-55	J. M. Frankovich	
DCL-83	Interpreted Instruction Code of the MIT CS II Computer	6-24-55	J. M. Frankovich	
DCL-84	The MIT Comprehensive System of Service Routines	6-27-55	P. C. Helwig	
DCL-88	Normal S & EC Operating Procedures	7-15-55	P. C. Helwig	
DCL-89	Recent Changes in the CS Conversion Program	7-15-55	J. M. Frankovich	
DCL-90	Whirlwind Display Program: Vibrations in a Length of String	6-17-55	D. N. Arden and G. W. Patterson	
DCL-91	Modification of the Numerically-Controlled Milling Machine Translation Routine for Use with the G&L Machine	7-19-55	A. Siegel	
DCL-92	Proposed Additional Function for the Read-In Button	7-22-55	F. C. Helwig	
DCL-94	Polynomial Factorization	8-1-55	M. Jacobs	
DCL-94-1	Revision in Polynomial Factorization	8-17-55	M. Jacobs	
DCL-97	Whirlwind I Processing Routine for Course 6.601	8-18-55	A. Siegel	
DCL-101	Iterative Solution of Linear Systems Having Sparse Matrices	9-12-55	M. D. McIlroy	

APPENDIX

4. 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, 11 groups totalling 253 people visited the computer installation. Included in these groups were:

June 28	Training Course for Whirlwind I
July 6	MIT Foreign Students Summer Project
July 11	Course in "Machine-Aided Analysis"
August 3	Westinghouse Science Teachers Project
August 29	Training Course for Whirlwind I
August 31	Summer Session Course in "Numerical Control of Machine Tools."
September 9	MIT Textile Department
September 13	MIT Freshmen
September 22	Worcester Polytechnic Institute Seniors

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 35 persons visited the Laboratory at the Open House demonstrations. These persons represented members and friends of the MIT community, Boston University, Harvard University, Tufts College, Royal Canadian Air Force, Michigan Department of Revenue, Arenberg Laboratory, and the University of Illinois.

During the past quarter there were also 43 individuals who made brief tours of the computer installation at different times. Represented by these individuals were Reliance Electronics and Engineering Co., Caswell Aeronautical Laboratory, U. S. Army Ordnance, Pratt and Whitney Aircraft Co., Convair, and the Air Force Armament Center.

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MACHINE METHODS OF COMPUTATION AND NUMERICAL ANALYSIS

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PROJECT WHIRLWIND

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