Digital Computer Laboratory
Massachusetts Institute of Technology
Cambridge 39, Massachusetts

SUBJECT: PROGRESS REPORT, SEPTEMBER 6 THROUGH OCTOBER 3, 1954

To: Jay W. Forrester

From: Scientific and Engineering Computation Group

1. MATHEMATICS, CODING AND APPLICATIONS

1.1 Introduction

During the four week period covered by this report, 534 coded programs were run on the time allocated to the Scientific and Engineering Computation (S&EC) Group representing work that has been carried on in 27 problems.

Section 1.2 contains progress reports as submitted by the programmers together with an indication of the machine time (and, in some cases, of the programming time) expended on each problem.

Additions to the CS II vocabulary are described under problem 100 for facilitating the use of director tapes. Requests for automatic curve plotting may now be used with CS II. The procedures are described in detail by N. Saber in Memorandum DCL-11.

Initial descriptions are provided below for problem 202 on the calculation of a vertical antenna coverage skeleton and for problem 204 on the exchange integrals between real Slater orbitals. This latter problem is being carried out in cooperation with the Department of Physics at the University of Chicago. Problem 202, carried out by A.F.Bartholomay of Lincoln Laboratory, was completed during this report period.

The next introductory coding course will be offered daily from 2-4 PM in room 1-150 for the two week period October 18-29. Attendance at this course is limited to those who are programming or are about to program an approved S&EC problem.

1.2 Programs and Computer Operation

100. The Comprehensive System of Service Routines: Arden, 38 hours; Best, 14 hours; Frankovich, 16 hours; Porter, 1 hour; Siegel, 49 hours; WWI, 1235 minutes

A new instruction, STOP (and iSTOP), will be added to the CS II vocabulary. This instruction is intended to provide a uniform method for ending programs and should replace the instructions presently used for this purpose (e.g., si0, sil, sp26, etc). STOP has the following functions:

If no director tape is being used the instruction sp(x+1), where x is the address of the register containing the STOP instruction, is stored in register 2 and the computer stops in register 1 (provided the stop on sil switch is on). If a director tape is being used, however, computer control goes to the utility control program which reads in the next word from the director tape.

The director tape section of the utility control program has been rewritten to operate from group 2 of the buffer drum since space for the program is no longer available on group 11. Two new director words have been added namely,

isa x	Start the program by interpreting the instruction contained in register x.
irs	Start the program by interpreting the instruction at register x+1, where x is the contents of the interpretive subroutine PC.

The new output blocks for automatic curve plotting on the scope have been tested and are now available for routine use.

120 D. The Aerothermopressor. Porter, 1 hour; Gavril, 160 hours; WWI, 384 minutes

The study of the fourth-order Runge-Kutta method for solving the differential equations of the aerothermopressor process has been completed, and it has been found that the intolerable error of ten per-cent in the final pressure computed by the Euler method can be reduced better than a hundredfold by this higher order method in about twice the computational time.

In addition to the quantitative data furnished by this study, much has been learned of a general nature which will be helpful in the planned revision of the aerothermopressor program as well as in interpreting further numerical results. It is believed that the following two facets of the study are of particular significance:

a) Nature of Accumulated Error-- With a fourth order method such as the one used, it had been expected that all errors would be a linear function of the fourth power of the increment size. However, such was not always found to be the case for all of the variables of the process. The results of the study indicate that in the case of simultaneous differential equations of the form

$$y_1' = f_1(x, y_1, y_2, y_2', y_3, y_3', \ldots)$$

$$y_2' = f_2(x, y_1, y_1', y_2, y_3, y_3', \ldots)$$

etc.

only those variables which are determined from equations involving as derivatives only the derivative of the variable in question, i.e., of the form

$$y_1' = f(x, y_1, y_2, y_3, \ldots)$$

will exhibit the expected variation of error with increment size, that is, vary linearly with $(\Delta x)^4$. The remaining variables (for example, the area of the duct in which the first derivative is a linear combination of derivatives of other properties of the flow) exhibit errors of lower order, and in some cases these are linear in the increment size Δx.

b) Scale of Error--The transition from the comparatively crude Euler method to the Runge-Kutta method resulted in such a significant reduction of truncation error that several heretofore latent and umimportant anomalies in the computations became a significant fraction of the error. For example, the substitution of the wet-bulb temperature of the stream for that of the liquid (for eliminating instability of the solution), though tenable from physical considerations in every case, was directly reflected in the Runge-Kutta solution by anomalous behavior of the error. Such difficulties were not observed with the Euler method since they were completely swamped out by truncation error. Another by-product of the study was the detection of several inconsistencies in distinguishing between differentials and increments of dependent variables.

The current subroutines will be used to continue calculations of aerothermopressor performance while the new program is being written. It is planned to make use of the design method described in the biweekly report of June 14, 1954 in attempting to determine the Mach Number variation for best performance of the aerothermopressor. Since the WWI program for this method cannot now be used, the necessary constants of the problem will be computed by hand.

126 C. Data Reduction: WWI, 360 minutes

During this period many tests were run on the Basic Data Reduction and previous versions, both with and without the Mistake Diagnosis Routine, to try to make the Basic version converge as well as the previous (second) version had. Various special techniques were tried to no avail. In the process, it was discovered that a copying error had been made in an early correction to the second version (an iad instead of an isu) which made it earier for the second version to converge. The error made so little difference in any one quantity that it was not detected in comparisons with hand computation, but it was found when two supposedly equivalent MDR results were compared. It now appears that further refinements must be made in one of the tabulated functions, the inverse of another tabulated function. Newton's method will be used to solve for equally spaced values to seven decimal places and a new polynomial for use in the Data Reduction Programs will be fitted by the Polynomial Fit Program.

An initial routine using auxiliary in-out equipment is being checked out and, when operative, will be combined with the Data Reduction Programs to allow monitoring, intervention, etc.

A logging routine is planned to record on magnetic tape pertinent information during the operation of the combined programs.

The large letter display routine is working. The large letters are roughly four times the size of the figures on scope post-mortems.

132 C. Subroutines for the Numerically Controlled Milling Machine. Runyon, 10 hours; WWI, 15 minutes

The only activity on the problem this month was the making of two runs for checking milling machine tapes. Programming for tape preparation will be resumed after November 1, 1954.

167 D. Transient Effects in Distillation. O'Donnell, 160 hours; WWI, 978 minutes

During the past period most of the effort was devoted to batch distillation. A small amount of computer time was used on the problem of transients in continuous distillation.

The work on transients in continuous distillation was preparatory to a more intensive attempt to correlate the data for a step change in reflux ratio. A limited amount of the data for concentrations versus time previously calculated on the machine was used to calculate more complicated functions. The work of correlating the more complicated functions has not proceeded far enough yet for evaluation.

The bulk of the machine time was used on batch distillation. The objective was to determine the overall effect of holdup in batch distillation, including the effects in both the equilibration and take-off periods. As normally operated, a batch distillation column has some holdup. After charging the stillpot with liquid, the column is normally put into operation at total reflux (no product take-off) for some time. This equilibration period requires a certain amount of vapor (disadvantageous) but increases the concentration of the holdup in the column so that the first product taken off is more concentrated than it would have been otherwise (advantageous). Also, during the product take-off period, the product concentration is higher the more vapor consumed during this period per unit of product removed. Actually, taking a case with a fixed ratio of holdup to charge, it is expected that for obtaining specified product concentration and amount, there will be some optimum combination of vapor consumption during the equilibration and take-off periods, giving a minimum total vapor consumption. It is also expected that if the ratio of holdup to charge is permitted to vary, there will be some optimum ratio of holdup to charge as well. Physical intuition leads to the expectation that the optimum ratio of holdup to charge will be zero, that is, no holdup. However, this cannot be achieved in practice. It is of interest to check whether this physical intuition is correct. It is also of interest to get an idea what the optimum methods of operation are for given ratios of holdup to charge and how much the total vapor consumption is affected by holdup. In order to get some specific answers to these questions the following program was carried out.

One mixture with one value for feed composition and relative volatility was studied, using a single column with a stillpot and five theoretical plates. Four different ratios of holdup to charge were used. First computations were made for the equilibration at total reflux in batch distillation starting with all the charge in the stillpot and continuing until the column was very near equilibrium.

Next values of concentrations in the column were taken from the preceding results for four different degrees of equilibration for each value of holdup-to-charge ratio. These were used as starting points for batch-distillation-take-off computations on the machine. Each starting point was run with two conditions for vapor consumption per unit of product during take-off (values of reflux ratio of three and ten). Thus a total of thirty-two of these cases were required.

About fifteen computations were done for the no-holdup case, where only take-off is done. These were for different values of vapor consumption per unit of charge distilled.

All of these computations were done on WWI. Existing programs were satisfactory for all the computations except the equilibration at total reflux. In this case a program originally written by Myers had to be revised and trouble-shot in order to get satisfactory results.

At present analysis of these data to determine answers to the questions mentioned above is taking place.

183 D. Blast Response of Aircraft. Porter, 2 hours; Shulman, 80 hours; WWI, 306 minutes

Programs III and IV which were started during the previous four week period were test run successfully and are ready for production runs.

During this period another program (V) was programmed and test-run successfully. It is essentially program IV simplified by considering the quasi-steady damping forces acting on the airplane instead of the unsteady ones. Results obtained from programs IV and V were compared, and since the simplifications of program V resulted in excessively large errors, this program was discarded in favor of the slightly longer, but much more accurate program IV. Production runs were carried out with program IV and the initial parametric study is now almost completed.

A new subroutine was added during this period for the purpose of determining the lethal criterion. It was test-run successfully and will be used for production runs to be done soon after the initial parametric study is completed.

184 C. Scattering of Electrons from Hydrogen. Newstein, 80 hours; WWI, 525 minutes

During the past period, final runs have been performed on a series of program, including several three dimensional integrals. The results check to the required accuracy for special values of the parameters.

195 C. Intestinal Motility. WWI, 120 minutes

Problem 195 involves about 100 sets of human intestinal motility data to be autocorrelated and the corresponding results transformed. The programs being used are the autocorrelation and Fourier transform programs developed by D.T.Ross under problem 107.

During the last month 50 sets of data were autocorrelated using a total of about 100 minutes, an average of 2 minutes per run. The significance of the results cannot be discussed until more data is correlated and the transforms computed.

To facilitate the processing of results, the automatic scope display routines are being incorporated into both of the programs. This modification will eliminate the need for plotting by hand the 101 points for each set of data.

199 C. Laminar Boundary Layer of a Steady, Compressible Flow in the Entrance Region of a Tube. Toong, 3 hours; WWI, 169 minutes

The required interval for the solution of the second set of differential equations by means of Gill's method was determined.

A solution was obtained for the second set of differential equations for the adiabatic case of an entrance Mach number of 2.8. This represents about another 1% of the entire job to be done by WWI.

Similar programs are to be run for various entrance Mach numbers and thermal conditions at the tube wall.

202 C. Calculation of Vertical Antenna Coverage Skeleton. Johnson, 160 hours; WWI, 17 minutes

A program has been developed for obtaining the "skeleton structure" of one such radiation pattern which consists of axes through the center of all lobes and loci of all null points for constants point differences. A more detailed explanation of the physical meaning of this problem can be found in a report now being written by A.F.Bartholomay of Lincoln Laboratory.

Using the (24,6) system a test program for this problem was run off successfully. After making revisions in the basic program, a run was made to obtain a pattern of thirty lobe lines for a fixed antenna height. This revised program printed out in decimal form the x and y coordinates for each point of the lobe lines and for the curve of the surface of the earth and, at the same time, using the automatic scope display subroutine, gave a scope display of the entire skeleton structure on one frame.

The successful completion of this last run terminates the problem. This decision has been reached, since further investigation reveals subtleties and complications in the problem itself, which make any continuation wasteful and unproductive to both programmer's and the computer's time.

204 C. Exchange Integrals Between Real Slater Orbitals WWI, 18 minutes

This problem involves the computation of the electrostatic interaction of two charge densities $\Omega(1)$, $\Omega(2)$ by Coulomb's Law.

$$\int \frac{\Omega(1)\,\Omega(2)}{r_{12}}\, dV_1\, dV_2$$

where the volume integrations are over all space. Each charge distribution is the product of two functions

$$x\,(\underbrace{n,\ l,\ m,\ \zeta,}_{\text{parameters}}\ \underbrace{r,\ \theta,\ \phi}_{\text{variables}})$$

$$= (2\zeta)^{n+\frac{1}{2}}/\left[\pi(2n)!\right]^{\frac{1}{2}}\ r^{n-1}\ e^{-\zeta r}\ \left[\frac{(2\ell+1)(\ell-m)!}{2(\ell+m)!}\right] P_\ell^M(\cos\theta).$$

$$\begin{cases} 1/\sqrt{2} & m = 0 \\ \left.\begin{matrix}\cos m\phi \\ \sin m\phi\end{matrix}\right\} & m \neq 0 \end{cases}$$

where the parameter ranges are $\ell+1 \leqq n$.

$m \leqq \ell$, and $\zeta \geqq 0$. The two functions whose product makes a charge distribution are located on a different center of two distinct centers.

The x and y axes of the two centers are parallel, the z axes are anti-parallel and coincide. The distinctness of the two centers introduces a final parameter the distance between the two centers, R.

A transformation of the variables to elliptic coordinates is effected and $\frac{1}{r_{12}}$ expanded in these coordinates in what is known as the Neumann expansion.

The resulting integral can be separated allowing the construction of an infinite series of integrals where the quadrature has been reduced from a six-fold to a double quadrature, the limit of the first quadrature being the argument of the second.

$$I = h \sum_{\ell = M}^{\alpha} I_{\ell}^{M}$$

$$I_{\ell} = K \int_{1}^{\alpha} d\xi (\xi^2 - 1)^{-1} f^{M}(\xi, \alpha) f'^{M}(\xi, \bar{\alpha})$$

α is a function of the ζ's arising from $\Omega(1)$ and R. $\bar{\alpha}$ is similarly defined for $\Omega(2)$.

$$f^{M}(\xi, \alpha) = \frac{1}{P_{\ell}^{M}(\xi)} \int_{1}^{\xi} dx\, P_{\ell}^{M}(x)(x^2-1)^{\frac{M}{2}} e^{-\alpha x} W_{\ell}^{M}(B,x)$$

where $W_{\ell}^{M}(B,x)$ is a polynomial in integral powers of x the coefficients of which are determined as functions of all the parameters arising in a given charge distribution.

The coefficients arising in the $W_{\ell}^{M}(B,x)$ polynomials are constructed from a set of Spherical Bessel functions of imaginary argument and $\frac{1}{2}$-integer order. Two arguments will be necessary for each total integration, and the process is to be carried out only once during the computation of a total integral.
From these Bessel functions further functions will be constructed with the construction of each I_{ℓ} by means of a simple recursion. At the outset it will be necessary to construct a table of coefficients. This table is representative of the multiplication of the two x functions together. The major portion of the computation is the numerical quadrature necessary to obtain an I_{ℓ}. The integration from 1 to ∞ is converted to an integration from 1 to 0, to give a finite range to the integration. The procedure will be to evaluate the integrand (including the inner integrations) exactly and approximate the outer integration by some "numerical quadrature" procedure.

To date the initial coefficient table - to be used in constructing the $W_{\ell}^{M}(B,x)$ polynomial has been coded by P. Merryman and is now being tested.

In view of the fact that the heaviest portion of the computational labor is in the numerical integration, repidly converging "numerical quadratures" schemes have been investigated. Of these schemes the most powerful - Gaussian, has proved adaptable, mutatus mutandis, and gives promise of decreasing the total necessary computation by the order of seventy percent of those necessary when using Simpson's Rule. This scheme has been flow-diagrammed for our specific case, and will shortly be coded and tested.

A subroutine giving spherical Bessel functions of imaginary argument and $\frac{1}{2}$ integer order, as well as square roots and exponentials, in (24,6) has been completed and tested by F.J.Corbató and is now ready for incorporation into this scheme.

The procedure for computing an exchange integral is now sketched in sufficient detail. The remaining effort will be almost entirely devoted to the tasks of coding, testing and assembly. We will report later upon the effectiveness of the quadrature procedure - at that time describing in detail the mathematical apparatus.

As reference for this problem see the Journal of Chemical Physics, Vol. 19, No. 12, 1459-1477, December 1951. "A Study of Two-Center Integrals Useful in Calculations on Molecular Structure. II The Two-Center Exchange Integrals " Klaus Ruedenberg.

207 C. Check for REAC. Mahoney, .5 hour; Porter, 3.5 hours; Larson, 40 hours; Whalen, 40 hours; WWI, 161 minutes

The main part of the program is now ready; we are experimenting with different interval sizes.

The following programs used computer time but did not report:

106 C.	MIT Seismic Project	61 minutes
123 C.	Earth Resistivity Interpretation	426 minutes
141.	S&EC Subroutine Study	17 minutes
143 D.	Vibrational Frequency Spectrum of a Copper Crystal	87 minutes
155 D.	Synoptic Climatology	370 minutes
159 D.	Water Use in a Hydroelectric System	1008 minutes
162 C.	Determination of Phase Shifts from Experimental Cross-Sections	3 minutes
166 C.	Construction and Testing of a Delta-Wing Flutter Model	118 minutes

173.	Course 6.537 Digital Computer Application Practice, Spring 1954	38 minutes
179 C.	Transient Temperature of a Box-Type Beam	27 minutes
180 B.	Crosscorrelation of Blast Furnace Input-Output Data	16 minutes
190 D.	Zeeman and Stark Effect in Positronium	71 minutes
191 B.	Earthquake Epicenter Location by Geiger's Method	23 minutes
193 C.	Eigenvalue Problem for Propagation of E.M.Waves	45 minutes
200 C.	A Study of Recurrent Events	124 minutes
201 C.	Study of the Ammonia Molecule	18 minutes
208 C.	Interceptor Flight Control Problem	21 minutes
209 A.	Numerical Solution of Homogeneous Linear Differential Equations with Quadratic Polynomial Coefficients	71 minutes
210 A.	Residue-Indices and Primitive Roots	34 minutes
211 C.	Servo Response to a Cosine Pulse	20 minutes
213 .	Industrial Process Control Studies	6 minutes

1.3 Operating Statistics

1.31 Computer Time

The following indicates the distribution of WWI time allocated to the S&EC Group during the four week period covered by this report.

Programs	114 hours, 52 minutes
Conversion	02 minutes
Magnetic Drum Test	1 hour , 45 minutes
Magnetic Tape Test	1 hour , 54 minutes
Scope Calibration	1 hour , 04 minutes
Total Time Used	119 hours, 37 minutes
Total Time Assigned	129 hours, 23 minutes
Usable Time, Percentage	92%
Number of Programs	534

2. COMPUTER ENGINEERING

2.1 WWI System Operation

(A.J.Roberts, L.L.Holmes)

The percent reliability of the computer system decreased considerably during the recent biweekly period. The down time was the result of diverse troubles. Some of the failures are as follows:

(1) Three incidents of undersized fusing of new power wiring;

(2) One case of improper checkout of completed computer modifications;

(3) A Freon leak in the newly installed piping for the modifications to the Room 222 air-conditioning system;

(4) An intermittently open video cable resulting in the erratic clearing of the A-register;

(5) A loose power connection resulting in improper displays;

(6) A faulty 5687 tube used as a cathode follower causing the undesirable selection of the mechanical reader whenever other input-output equipment was being used.

(7) Two core-memory parity alarms due to a fault with the sensing amplifiers.

As a result of the above troubles, several corrective measures have been taken. The engineers and technicians have been reminded of the standard procedures required for new installations and modifications. Technicians who are on duty whenever troubles occur have been requested to spend less time by themselves fixing the failure and to seek the assistance of a system engineer after a reasonable time of trouble-shooting has elapsed. The core-memory sensing amplifiers have been modified to correct for excessive grid current present in some stages. The strobe pulse for core memory was increased in amplitude.

2.2 Terminal Equipment

Magnetic Drums
(H.L.Ziegler)

A chapter entitled "Erasing the WWI Magnetic Drums" has been written and submitted as part of the "Magnetic Drums Technician's Manual".

The magnetic-drum Mod II test rack is now complete and is in full-time use. Efficiency and convenience of chassis testing is considerably improved over that of the Mod I test rack.

Test Programs
(D.A.Morrison)

The following WWI Test Programs have been modified for use with the new sequence of flip-flop storage registers:

T-3432 Consolidated Test Program
T-3218-21 Arithmetic Element Check
T-3372 Magnetic Tape Test

Modification of the other commonly used test tapes was not necessary.

3. ADMINISTRATION AND PERSONNEL

New Staff

Bernard Riskin has joined Group 6345 as a part-time staff member. He has a B.S. from Temple University in Philadelphia.

Staff Terminations

Malcolm Demurjian

4. RECENT LIBRARY ACQUISITIONS

The following documents have been recently acquired by the Barta Building Library, Room 109.

No.	Title	Source
C-172	Design and Operation of Digital Calculating Machinery -Progress Report May-August, '54	Harvard University
C-173	Program Library Index	Univ. of Illinois
C-174	On the Choice of Mesh in the Integration of Ordinary Differential Equations	Ballistic Research Laboratories
C-175	The Improvement of Accuracy in Integration	Ballistic Research Laboratories

The following is a list of all DCL memos to date. Copies may be obtained from the Barta Building Library, Room 109.

No.	Title	Author
DCL-1	Procedure for Memos Issued by S&EC Group	C.W.Adams
DCL-2	Making Electrons Count	C.W.Adams
DCL-3	Biweekly Report, July 25, 1954	S&EC Group
DCL-4	Laboratory Personnel - Project 6345 1 August, 1954	
DCL-5	Table of Powers of 2	K. Ralston

No.	Title	Source
DCL-6	Progress Report, July 12 - August 8, 1954	S&EC Group
DCL-7	The "FL" Flexowriter Code Binary Numerical Sequence reprint of p.20 of M-1623	
DCL-8	The "FL" Flexowriter Code Alphanumerical Sequence reprint of p.19 of M-1623	
DCL-9	Biweekly Report, August 23, 1954	S&EC Group
DCL-10	Laboratory Personnel - Project 6345 September 1, 1954	
DCL-11	Automatic Scope Output Display Routines	N.J.Saber
DCL-12	A Program for Transferring Binary Information Back and Forth between Paper Tape and Magnetic Tape	S. Best
DCL-13	Progress Report, August 9-September 5,1954	S&EC Group
DCL-14	Biweekly Report, September 20, 1954	S&EC Group
DCL-15	S&EC Applications Problems	
DCL-16	Laboratory Personnel - Project 6345 October 1, 1954	
DCL-17	A Program for Checking the Contents of Test Storage	A. Siegel
DCL-18	Progress Report, September 6-October 3, 1954	S&EC Group