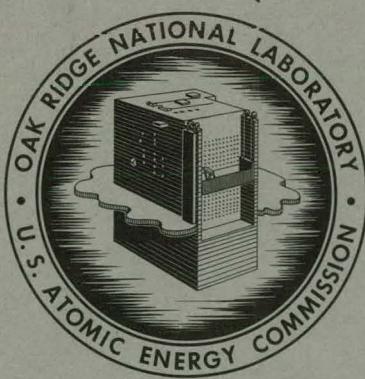


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ORNL-3423

**UC-32 – Mathematics and Computers**  
**TID-4500 (19th ed.)**

**MATHEMATICS DIVISION**  
**ANNUAL PROGRESS REPORT**  
**FOR PERIOD ENDING DECEMBER 31, 1962**



**OAK RIDGE NATIONAL LABORATORY**  
operated by  
**UNION CARBIDE CORPORATION**  
for the  
**U. S. ATOMIC ENERGY COMMISSION**

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ORNL-3423  
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Contract No. W-7405-eng-26

**MATHEMATICS DIVISION**  
**ANNUAL PROGRESS REPORT**  
**for Period Ending December 31, 1962**

A. S. Householder, Director  
A. C. Downing, Assistant Director

DATE ISSUED

APR 17 1963

OAK RIDGE NATIONAL LABORATORY  
Oak Ridge, Tennessee  
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# Numerical Analysis Research

A. A. Grau

## GENERALIZATION OF THE BAIRSTOW PROCESS

Iterative methods for solving polynomial equations generally make use at some point of algebraic divisibility properties of polynomials. Basic is the property that given two polynomials  $f(x)$  and  $g(x)$ , polynomials  $q(x)$  and  $r(x)$  may be determined so that

$$f(x) = q(x)g(x) + r(x). \quad (1)$$

Here  $q(x)$  and  $r(x)$  are called respectively the quotient and the remainder of the division of  $f(x)$  by  $g(x)$ . In order that they each be unique, it is customary to require that  $r(x)$  be of a degree lower than that of  $g(x)$ .

Instead of the above requirement, uniqueness may be obtained computationally by specifying the algorithm for determining  $q(x)$  and  $r(x)$ . Any algorithm which produces the correct quotient of the division of  $f(x)$  by  $g(x)$  when the former is exactly divisible by the latter, and which ensures that (1) holds, possesses all properties that are generally needed in the discussion of iterative methods. The examination of possible division algorithms other than the usual one, therefore, permits a generalization of any of the iterative methods for solving polynomial equations. This has been done in one instance.<sup>1</sup> It is instructive to do this more generally for the Bairstow process.

Let

$$f(x) = \sum_0^{n_f} f_i x^i, \quad g(x) = \sum_0^{n_g} g_i x^i, \quad q(x) = \sum_0^{n_q} q_i x^i,$$

the summations in all cases running over  $i$ . If  $f(x)$  is exactly divisible by  $g(x)$ , that is, if there exists  $q(x)$  so that  $g(x)q(x) = f(x)$ , then  $n_f = n_g + n_q$ , and

$$f_i = \sum_j g_j q_{i-j}, \quad i = 0, \dots, n_f, \quad (2)$$

where in each case the summation extends from the larger of 0 and  $i - n_q$  to the smaller of  $i$  and  $n_g$ . The system of  $n_f + 1$  equations (2) in the  $n_q + 1$  unknowns  $q_0, \dots, q_{n_q}$  may be solved for the latter;

<sup>1</sup>V. A. McAuley, "A Method for the Real and Complex Roots of a Polynomial," *J. Soc. Ind. Appl. Math.* **10**, 657-67 (1962).

in the case where  $f(x)$  is an exact multiple of  $g(x)$  the system is dependent, and  $n_g$  of the equations may be disregarded. However, when  $f(x)$  is not an exact multiple of  $g(x)$ , the same system is inconsistent; in this case different division algorithms may be obtained by disregarding different subsets of  $n_g$  of the equations.

A set of convenient division algorithms may be obtained as follows: disregard in (2) the equations involving  $f_k, f_{k+1}, \dots, f_{k+n_g-1}$ , and solve the remaining system for  $q_0, \dots, q_n$ . The polynomial  $r(x)$  in all cases may then be computed by (1). We may call the resulting algorithm  $A_k$ . A slight adaptation may be made if  $k > n_f$  or  $k < 0$  to include these cases also.

The Bairstow process as practically used requires two polynomial divisions for each iteration. If  $f(x)$  is the polynomial to be factored and  $p(x)$  is a trial quadratic factor, two divisions yield

$$f(x) = f_1(x) p(x) + r(x) , \quad (3)$$

$$f_1(x) = f_2(x) p(x) + s(x) . \quad (4)$$

A correction to the factor  $p(x)$  is then determined from the remainders  $r(x)$  and  $s(x)$ . The process generally studied makes use of the usual division algorithm  $A_0$  for carrying out both (3) and (4). The McAuley algorithm uses  $A_{n_f-2}$ .

The known properties of the standard Bairstow process and the McAuley process suggest how the convergence properties of the general Bairstow process may vary as  $k$  is varied from 0 to  $n_f$ . In addition, since it is possible to apply either the regular Bairstow or the McAuley algorithm to  $f(1/x)$  and  $p(1/x)$ , some insight into the behavior when two different algorithms are used for the two divisions (3) and (4) is also possible. The former is the general process using  $A_{n_f+1}$  and  $A_{n_f-1}$  and the latter is the general process using  $A_1$  and  $A_{-1}$ . From these considerations it becomes intuitively clear why the McAuley algorithm behaves much like the "inverse" regular Bairstow. They also lead to the conjecture that forms of the algorithm with  $k$  near  $n_f/2$  should prove useful in the case of equations with roots nearly equal in absolute value. This has been borne out by experiment.

## SPECIAL FUNCTIONS

Walter Gautschi

Recurrence relations are a valuable tool in the calculation of special functions. Their use leads to fast and compact computer programs. As with many recursive processes, however, the inherent possibility of instability demands considerable care. For linear first-order recurrence relations, and to some extent for second-order recurrences, an analysis of error propagation was made previously.<sup>2,3</sup> In the meantime the case of second-order recurrence relations has been investigated more thoroughly, and several examples — notably Bessel functions — have been examined in detail.

<sup>2</sup>Walter Gautschi, "Recursive Computation of Certain Integrals," *J. Assoc. Comput. Mach.* **8**, 21-40 (1961).

<sup>3</sup>Walter Gautschi, "Recursive Computation of the Repeated Integrals of the Error Function," *Math. Comput.* **15**, 227-32 (1961).

Let the recursion be

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0 \quad (n = 1, 2, 3, \dots),$$

where we assume that  $b_n \neq 0$  for all  $n$ . The coefficients  $a_n, b_n$  may depend on further parameters. Suppose  $f_n$  satisfies this relation, and is to be calculated for  $n = 0, 1, \dots, N$ . Let us also assume that there exists an identity

$$\sum_{m=0}^{\infty} \lambda_m f_m = s$$

with known  $\lambda_m, s$ . The possibility that all but one of the  $\lambda_m$  are zero is not excluded. Our concept of instability consists in assuming the presence of a second solution,  $g_n$ , which dominates for large  $n$ , in the sense

$$f_n/g_n \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

This forbids, in general, the use of the recurrence relation in the straightforward manner, since rounding errors inevitably introduce fractions of the dominant component  $g_n$ .

One method to eliminate the influence of  $g_n$  is to start the recurrence at  $n = \nu > N$ , with initial values  $y_{\nu+1} = 0, y_{\nu} = 1$ , and run through it in reverse direction, that is, in the order of decreasing  $n$ . The resulting sequence  $\{y_n^{(\nu)}\}$  will be approximately proportional to  $\{f_n\}$  in the interval  $0 \leq n \leq N$ , and the assumed identity may be used to determine the factor of proportionality. If  $f_n^{(\nu)}$  ( $n = 0, 1, \dots, N$ ) are the approximations so obtained, one shows that  $\lim_{\nu \rightarrow \infty} f_n^{(\nu)} = f_n$ , provided that

$$\lim_{\nu \rightarrow \infty} \frac{f_{\nu+1}}{g_{\nu+1}} \sum_{m=0}^{\nu} \lambda_m g_m = 0.$$

It should be noted that initial values  $f_0, f_1$ , in general, need not be known.

This method suffers from the fact that the numbers  $y_n^{(\nu)}$  generated by backward recursion may become extremely large, so as to cause overflow on a computer, even if floating-point arithmetic is used. This can be avoided by introducing the ratios

$$r_n^{(\nu)} = y_{n+1}^{(\nu)} / y_n^{(\nu)},$$

which obviously satisfy a nonlinear first-order recurrence relation. Knowing the ratios, we can obtain the  $y_n^{(\nu)}$  themselves, and thus also the  $f_n^{(\nu)}$ , by again using the assumed identity. The following is a convenient computational arrangement of this procedure:

$$\left. \begin{aligned} r_{\nu}^{(\nu)} &= 0, & r_{n-1}^{(\nu)} &= -b_n / (a_n + r_n^{(\nu)}) \\ s_{\nu}^{(\nu)} &= 0, & s_{n-1}^{(\nu)} &= r_{n-1}^{(\nu)} (\lambda_n + s_n^{(\nu)}) \end{aligned} \right\} \quad n = \nu, \nu - 1, \dots, 1;$$

$$f_0^{(\nu)} = s / (\lambda_0 + s_0^{(\nu)}), \quad f_{n+1}^{(\nu)} = r_n^{(\nu)} f_n^{(\nu)}, \quad n = 0, 1, \dots, N - 1.$$

It should be observed that the generation of the  $r_n^{(\nu)}$  amounts to evaluating the continued fraction

$$r_0^{(\nu)} = -\frac{b_1}{a_1} - \frac{b_2}{a_2} - \dots - \frac{b_\nu}{a_\nu}$$

from tail to head. It is known<sup>4</sup> that our condition of instability implies the convergence of the continued fraction as  $\nu \rightarrow \infty$ . It may also be noted that the  $y_n^{(\nu)}$ ,  $y_{n-1}^{(\nu)}$ , calculated previously, are the numerators and denominators, respectively, of this continued fraction.

This algorithm has recently been applied to the calculation of Bessel functions of the first kind and of arbitrary positive order. If  $f_n = J_{a+n}(x)$ , where  $0 \leq a < 1$ ,  $x > 0$ , then  $f_n$  is a solution of

$$y_{n+1} - [2(a+n)/x] y_n + y_{n-1} = 0 \quad (n = 1, 2, 3, \dots).$$

It is known<sup>5</sup> that

$$\sum_{m=0}^{\infty} \frac{(a+2m) \Gamma(a+m)}{m! \Gamma(1+a)} f_{2m} = (\frac{1}{2} x)^a / \Gamma(1+a);$$

therefore we may take

$$\lambda_0 = 1, \quad \lambda_{2m} = \frac{(a+2m) \Gamma(a+m)}{m! \Gamma(1+a)}, \quad \lambda_{2m+1} = 0, \quad s = (\frac{1}{2} x)^a / \Gamma(1+a).$$

A second solution is  $g_n = Y_{a+n}(x)$ , and we have

$$f_n \sim (e^{-a} / \sqrt{2\pi n}) (ex/2n)^{a+n}, \quad g_n \sim -e^a \sqrt{2/\pi n} (2n/ex)^{a+n} \quad (n \rightarrow \infty),$$

so that indeed  $f_n/g_n \rightarrow 0$  very quickly, as  $n \rightarrow \infty$ .

It would be tempting to use the same identities for the calculation of

$$f_n = I_{a+n}(x) = e^{-i(a+n)\pi/2} J_{a+n}(ix),$$

by making the substitution  $x \rightarrow ix$  throughout. The resulting procedure, however, turns out to be satisfactory only for small or moderately large values of  $x$ , while for large  $x$  serious loss of accuracy is encountered. The reason for this may be found in the fact that for large  $x$

$$\lim_{\nu \rightarrow \infty} (\lambda_0 + s_0^{(\nu)}) = \frac{s}{f_0} \sim \frac{\sqrt{2\pi}}{\Gamma(1+a)} 2^{-a} x^{a+1/2} e^{-x},$$

which is a small quantity. Since  $\lambda_0 = 1$ , this means that in calculating  $f_0^{(\nu)} = s / (\lambda_0 + s_0^{(\nu)})$  serious cancellation must occur.

To avoid this difficulty we chose another identity, namely,<sup>6</sup>

$$2^a \Gamma(a) \sum_{m=0}^{\infty} (m+a) C_m^a(\gamma) I_{a+m}(x) = x^a e^{\gamma x},$$

<sup>4</sup>Oskar Perron, *Die Lehre von den Kettenbrüchen*, vol II, p 97, B. G. Teubner, Stuttgart, 1957.

<sup>5</sup>G. N. Watson, *A Treatise on the Theory of Bessel Functions*, 2d ed., p 138, Cambridge University Press, 1958.

<sup>6</sup>Arthur Erdélyi et al., *Higher Transcendental Functions*, vol II, p 98, McGraw-Hill, New York, 1953.

where  $C_m^a(\gamma)$  are Gegenbauer polynomials. Letting  $\gamma = 1$ , and rewriting it in a more suitable form, one is led to an identity with

$$\lambda_0 = 1, \quad \lambda_m = 2 \frac{(a+m) \Gamma(2a+m)}{m! \Gamma(1+2a)} \quad (m \geq 1), \quad s = (\frac{1}{2}x)^a e^x / \Gamma(1+a).$$

We now have, when  $x$  is large,

$$\lim_{\nu \rightarrow \infty} (\lambda_0 + s_0^{(\nu)}) \sim \frac{\sqrt{2\pi}}{\Gamma(1+a)} 2^{-a} x^{a+1/2},$$

so that the danger of cancellation is effectively removed.

In using these procedures on a digital computer, it is very desirable to have reasonably good estimates for the initial value  $\nu$  of  $n$ , given the number  $d$  of significant digits desired. In the case of Bessel functions such an estimate may be found in the form

$$\nu \geq \max \left[ Nt \left( \frac{D}{2N} \right), \frac{e}{2} x t \left( \frac{2D}{ex} \right) \right]$$

for  $J_{a+n}(x)$ , and in the form

$$\nu \geq \begin{cases} \max \left[ Nt \left( \frac{D}{2N} \right), \frac{e}{2} x t \left( \frac{2(D-x)}{ex} \right) \right] & \text{if } x < D, \\ \max \left[ Nt \left( \frac{D}{2N} \right), \frac{e}{2} x \right] & \text{if } x \geq D, \end{cases}$$

for  $I_{a+n}(x)$ . Here,  $D = d \cdot \ln 10 + \ln 4$ , and  $t(y)$  denotes the inverse function of  $y = t \ln t$  ( $t \geq 1$ ). A sufficiently accurate approximation to  $t(y)$  may be obtained by a Taylor expansion about  $y = 0$ , when  $y$  is small, by a least-squares approximation, when  $y$  is moderately large, and by the approximation formula

$$t(y) \approx \frac{y}{\ln y} \frac{1}{1 - (\ln \ln y)/(1 + \ln y)},$$

when  $y$  is large.

To give another example, consider the integrals

$$f_n = \frac{(-1)^n}{2} \int_0^\pi \left(1 - x \sin^2 \frac{t}{2}\right)^a \cos(nt) dt \quad (0 < x < 1),$$

where  $a$  is any real number. For  $a = -5/2$ , these integrals are of interest in airfoil theory.<sup>7</sup> One shows that they are a solution of

$$y_{n+1} - \frac{2n}{n+a+1} \frac{2-x}{x} y_n + \frac{n-a-1}{n+a+1} y_{n-1} = 0 \quad (n = 1, 2, 3, \dots),$$

<sup>7</sup>J. Siekmann, "Concerning an Integral Occurring in Airfoil Theory," *Soc. Ind. Appl. Math. Rev.* **3**, 243-46 (1961).

which is a Poincaré difference equation, that is, its coefficients have definite limits as  $n \rightarrow \infty$ . From Poincaré's theory<sup>8</sup> it can be concluded that there is one solution that decreases geometrically, and another that increases geometrically. Since  $f_n$  are Fourier coefficients of a smooth function, we have  $f_n \rightarrow 0$ , so that  $f_n$  may be identified with the decreasing solution. With  $g_n$  any other solution, we then obviously have  $f_n/g_n \rightarrow 0$  as  $n \rightarrow \infty$ , that is, instability. By Fourier expansion techniques one can find the following identity to be used for scaling:

$$f_0 - 2 \sum_{m=1}^{\infty} \frac{f_{2m}}{4m^2 - 1} = \frac{\pi}{2} \frac{1 - (1 - x)^{\alpha+1}}{(\alpha + 1) x}.$$

---

<sup>8</sup>Henri Poincaré, "Sur les équations linéaires aux différentielles ordinaires et aux différences finies," *Am. J. Math.* 7, 213-17, 237-58 (1885).

## Medical and Biological Statistics

M. A. Kastenbaum    D. G. Gosslee    D. A. Gardiner  
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The statistical services in the field of biology and medicine cover a broad area which, with few exceptions, involves all the fields of fundamental research engaged in by the Biology Division. The basic services in all these fields consist of constructing and testing mathematical models, developing procedures for estimating mortality intensity, fitting multihit survival curves, and estimating the median lethal dose ( $LD_{50}$ ) for various types of organisms irradiated with various forms of radiation. Standard statistical techniques such as the analysis of variance, regression analysis, and confidence-interval estimation were used wherever applicable. In addition, wherever possible, new techniques were developed to handle problems which were not of a routine statistical nature.

A much greater emphasis was placed this year on the use of high-speed computers for handling large quantities of data which previously might have been unmanageable. Also, many areas of investigation such as testing new mathematical models in biology were attempted because the availability of computers made the solution of such problems attainable. In some cases new mathematical models to describe biological situations were derived with the help of the investigator by use of a probability argument. All models so derived and all existing models were tested against experimental data by use of the high-speed computers. In one instance, at least, the statistician was able to point out a slight flaw in the investigator's interpretation of the biological phenomena and thus adjust the mathematical model to better suit the biology involved.

In 1962 great emphasis was placed on the design of experiments in the statistical sense. Several experiments in biology, at least one of which is described below, were designed using response surface methodology. In so doing it was demonstrated how a response which is a function of more than one variable may be handled with a minimum of effort by the investigator if some prior thought is given to an appropriate experimental design. The use of this technique pointed up very clearly how a little prior planning of an experiment could accomplish the same results with one-fifth the experimental material.

Discussions continued and plans were laid for the long-range low-level-radiation study to be carried out by the Biology Division. Decisions were made concerning the numbers of mice required to detect small differences due to irradiation at low levels, and to provide information concerning myeloid leukemia through ancillary serial sacrifice studies.

Finally, a small study of the death rate among employees at ORNL was started jointly with the Health Division. This study, which is being carried out with the cooperation of the Bureau of Old Age and Survivor's Insurance, is still in its earliest stages. Some results should be forthcoming within the next report period.

### **BIOMEDICAL-DATA RECORDING**

The use of IBM cards for recording biological data was accentuated during this report period. In addition to the increased numbers of problems which were processed for the Biology Division, such jobs as handling the Health Physics Division's pocket-ionization-chamber data could be accepted and placed on a routine basis. The capacity of the data-recording unit to expand its scope was enhanced by the addition to the staff of one key-punch operator in July 1962. In anticipation of an increasing demand for these services, an IBM 557 alphabetic interpreter and a second IBM 026 card punch were ordered. Delivery is expected during the first half of 1963.

Among the many jobs handled by the data-recording unit in 1962, the following are some of the more important:

1. Cytology and Genetics

- (a) Paramecium mutation. The number of cards punched for this section continues at about 200 per week. These cards are processed weekly on the IBM 7090 system at ORGDP.
- (b) Drosophila. Information from these experiments is punched on a routine basis, and then processed on the IBM 1401 system at the Y-12 Plant. Tabulations are made by class, container, and day within each experiment. From class counts, ratios for male and female viability and nondisjunction are shown.

2. Mammalian Genetics. Results from one extensive experiment were punched on cards. This experiment was a study of mutation in sperm after males were subjected to 300-r x-ray doses. Approximately 30,000 cards for this experiment have been punched.

3. Mammalian Recovery

- (a) Hemopoietic recovery. The backlog of data relating to "old" experiments of bone marrow studies was eliminated. Various tabulations and summaries of results were made to expedite further statistical evaluations.
- (b) Tissue culture. Preliminary discussions have taken place with a member of the group for establishing a method of storing and retrieving publication references in his area of interest.

4. Pathology and Physiology

- (a) Pathological effects of radiation. Records of animal autopsies and cataract studies, including those for experiments up to the present, were transferred to punched cards. Tabulations and summaries of these data have been made.
- (b) Physiological and chemical effects. Conferences were held with an investigator of this section to plan the recording of experimental results on cards.

## 5. General (Biology Division)

- (a) A title and author card are punched for each journal reference cited in the weekly bulletin of the Biology Division. At four-week intervals these cards are processed on the IBM 7090 system using the Bell Laboratories Permutation Index Program (BEPIP). Output for our purpose is a permuted title index and an author index on duplimat masters. A typical four-week set of cards thus yields a pamphlet of about 70 pages.
- (b) Work requests for maintenance from the engineering section of the Biology Division are now being processed by the data recording unit. The information is listed on the IBM 1401 system. Three weekly lists are produced as follows: (1) active work requests in work order number, (2) active work requests in craft order, and (3) completed work requests by work order number.

## 6. Health Physics Division

- (a) Applied health physics. Readings from pocket ionization chambers are being punched routinely since midyear. Weekly and quarterly listings are made on the IBM 1401, showing daily readings, weekly totals, and cumulative quarterly totals. In addition, limit violations are indicated.
- (b) Radiation ecology
  - 1. Approximately 5000 cards were punched from TVA Forest Mapping Service work sheets.
  - 2. A sample of about 4000 title cards of Biological Abstracts index was received. Corresponding author cards have been punched. A test run will be made in the near future using the BEPIP program.
  - 3. About 4000 cards were punched and listed relating to fish studies.
- 7. ORINS Biomedical Division. A small amount of amino acid data was processed on the IBM 1401. Approval for transfer of funds to continue this work has been obtained by ORINS.
- 8. Health Division. Portions of the employee records of approximately 2000 persons who have been terminated from ORNL since 1950 were punched onto IBM cards for further processing by the U.S. Bureau of Old Age and Survivor's Insurance in a cooperative effort of this agency with the ORNL Health Division.

## BIOPHYSICS

Normal and ultraviolet-irradiated deoxyribonucleic acids (DNA's) of several species were used as primers for DNA synthesis using calf-thymus polymerase, and the frequencies of the "nearest neighbors" have been determined in the product DNA. For each of the 27 DNA's considered, a system of four simultaneous homogeneous equations in as many unknowns was generated. Unique solutions for these sets of equations were attainable because of an added constraint on the unknowns. The observation matrix was a  $4 \times 4$  matrix, the first three rows of which were the coefficients of any three of the four observed equations; the elements in the last row represented the coefficients of the constraining equation. If  $A$  is the  $4 \times 4$  matrix so described and  $b$  is the  $4 \times 1$  column vector of the unknown parameters, then the matrix equation to be solved is

$$Ab = g,$$

where  $g^T = [0, 0, 0, 1]$ . The solution of the equations is given by

$$b = A^{-1}g,$$

where  $A^{-1}$  is the inverse of  $A$ . But  $A^{-1}g$  is given by the elements of the last column of  $A^{-1}$ . Thus the unique solution of the simultaneous equations is given by the elements of the last column of the inverse of the observation matrix.

The data from all 27 experiments were punched onto IBM cards in appropriate format for matrix inversion by the IBM 7090. To ensure uniqueness of the solutions (i.e., to detect any errors in transcription), each of the 27 sets was duplicated by eliminating a second observation equation different from the first. The resulting 54 matrices were inverted by the 7090 in less than 2 min.

## CELL PHYSIOLOGY

A number of experimental factors affect the survival of cells at low temperatures. Certain relationships between vapor pressure and temperature may be expressed in terms of the following differential equations:

Let  $V$  be vapor pressure and  $T$  be temperature, where  $V' = dV/dT$ ,  $V'' = d^2V/dT^2$ , and let  $k_1$ ,  $k_2$ ,  $k_3$ ,  $b$ ,  $r$ , and  $s$  be constants. Then

$$TV'' - V' = k_1, \quad (1)$$

$$T(T - b)V'' + bV' = k_2, \quad (2)$$

$$\frac{T}{r(T - b) - s} V'' - \frac{br + s}{[r(T - b) - s]^2} V' = k_3. \quad (3)$$

Each of these equations was integrated explicitly, with respective results

$$V = C_1 T^2 + k_1 T + C_3, \quad (1')$$

$$V = C_3[(T - b) + b \log(T - b)] + \frac{k_2 T}{b} + C_4, \quad (2')$$

$$V = \frac{k_3 r}{2} T^2 - k_3(rb + s)T + C_5, \quad (3')$$

where  $C_1$ ,  $C_2$ ,  $C_3$ ,  $C_4$ ,  $C_5$  are constants.

\* \* \* \* \*

The percentage survival of many cells to low-temperature exposure is increased by using low cooling velocities. Qualitatively, the increase is consistent with the view that slow cooling decreases the probability of intracellular freezing by permitting the cells to lose water at a rate sufficient to keep the protoplasm at its freezing point. The concern was to derive a quantitative relation between the amount of water in a cell and temperature. The resulting differential equation was solved numerically by the Runge-Kutta method, using values for the parameters applicable to specific cells, the important parameters being cooling rate, surface/volume ratio, permeability to water, and the temperature coefficient of the permeability

constant. The resulting calculated water contents were similar to those that have been observed experimentally and permitted predictions as to whether intercellular ice would be formed. The predictions are consistent with the experimental observations of several investigators.

## CYTOLOGY AND GENETICS

Irradiation of drosophila males may produce a shift in the ratios of the different genotypes recovered among the progeny. A method has been developed for treating progeny ratios, following paternal radiation, as the ratio of two survival functions, where survival refers to the ability of a mature sperm of a particular genotype to produce an adult fly in the next generation.

Consider a population of mature sperm composed of cells of different genotypes that occur with relative proportions  $\alpha_1, \alpha_2, \dots, \alpha_s$ , where  $\sum_{j=1}^s \alpha_j = 1$ . If the population is treated with various doses of radiation  $X_1, X_2, \dots, X_r$ , then the probability that, following the  $i$ th dose ( $i = 1, 2, \dots, r$ ), a sperm of the  $j$ th genotype will be able to produce a viable individual in the next generation may be expressed as  $S_{ij} = e^{-b_j X_i}$ , where  $b_j$  is the sensitivity constant of sperm of the  $j$ th genotype. The joint probability that a sperm will be of the  $j$ th genotype and will survive the  $i$ th dose is then  $Q_{ij} = \alpha_j e^{-b_j X_i}$ .

The experimental measure of  $Q_{ij}$  is  $n_{ij}/N_i$ , where  $n_{ij}$  is the number of surviving individuals resulting from fertilization by sperm of the  $j$ th genotype treated with the  $i$ th dose of radiation, and  $N_i$  is the total number of sperm sampled following  $X_i$ . Unfortunately, owing to the induced elimination of sperm from the irradiated sample prior to eclosion of the scored generation,  $N_i \neq \sum_{j=1}^s n_{ij}$ . Consequently we have no measure of  $N_i$  and thus none of  $Q_{ij}$ . If, however, we form the ratio  $Q_{ij}/Q_{i1}$ ,  $N_i$  drops out and we have

$$R_{ij} = \frac{Q_{ij}}{Q_{i1}} = \frac{n_{ij}}{n_{i1}} = \frac{\alpha_j}{\alpha_1} e^{-(b_j - b_1)X_i} = \alpha_j e^{-\beta_j X_i},$$

where  $\alpha_j$  represents the ratio of the  $j$ th sperm type to first sperm type in the initial population and  $\beta_j = b_j - b_1$  is a measure of the difference in sensitivity between sperm of the  $j$ th genotype and sperm of the first genotype.

Estimates of the unknown parameters  $\alpha_j$  and  $\beta_j$  may be achieved by the method of maximum likelihood as follows: Let  $p_{ij} = R_{ij}/\sum_{j=1}^s R_{ij}$ , so that  $\sum_{j=1}^s p_{ij} = 1$ . Then if  $T_i = \sum_{j=1}^s n_{ij}$  is the total number of individuals observed at dose  $i$ , the joint probability of observing  $n_{ij}$  individuals in the  $j$ th group out of a total of  $T_i$  individuals at dose  $i$ , for all groups and all doses, is given by

$$P = \prod_{i=1}^r \prod_{j=1}^s \frac{T_i!}{n_{ij}!} p_{ij}^{n_{ij}}.$$

Let  $L = \log P$  be the likelihood function. Then the solution of the equations  $\partial L/\partial \alpha_j = 0$  and  $\partial L/\partial \beta_j = 0$  will provide maximum-likelihood estimates of  $\alpha_j$  and  $\beta_j$ . These equations are highly nonlinear and cannot be solved explicitly. Particular solutions may be achieved numerically, however, for data from specific experiments by use of appropriately programmed high-speed computers. This was, in fact, done on the 7090 computer using a general nonlinear least-squares program.

If  $\hat{\alpha}_j$  and  $\hat{\beta}_j$  are the maximum-likelihood estimates of  $\alpha_j$  and  $\beta_j$  respectively (for  $j = 2, 3, \dots, s$ ), then  $\hat{R}_{ij} = \hat{\alpha}_j e^{-\hat{\beta}_j X_i}$  and  $\hat{p}_{ij} = \hat{R}_{ij} / \sum_{j=1}^s \hat{R}_{ij}$ . With this information the expected cell frequencies may be calculated as  $E(n_{ij}) = T_i \hat{p}_{ij}$ . Chi-square may then be applied to test the goodness of fit to the model. The number of degrees of freedom associated with this test is  $(r - 2)(s - 1)$ .

\* \* \* \* \*

Although the experiment to be described will be performed at San Diego State College, the design was formulated at ORNL while the investigator was a visiting scientist with the Biology Division. The purpose of the study is to quantitatively evaluate the functional relationship between survival of the first instar larvae of *Drosophila melanogaster* and dose and time of x irradiation.

A three-stage sequential design was selected because it provides an opportunity to approximate the relationship by a polynomial in successive steps of increasing complexity. The first stage allows for the fitting of a first-order polynomial; the first and second stages allow for the fitting of a second-order polynomial; all three stages provide the data for fitting a third-order polynomial. Between stages the investigator can decide to stop gathering data or to continue with the next stage, as he sees fit.

The experimental design is a third-order rotatable design of a type described by Gardiner *et al.*<sup>1</sup>. This is one of a class of designs devised for the fitting of response surfaces. At each point in the dose-time plane, 100 larvae will be irradiated. The arc sine of the square root of the survival population will be used as the dependent variable. The independent variables are within the range 600 to 1300 r for x irradiation and within the range 1 to 5 hr for time.

The first stage consists of five points in the two-dimensional factor space; the second stage consists of five points also; the third stage requires eight additional points. If the experiment runs to three stages, 18 points in total will be required. As a check on experimental error, the design will be replicated three times.

This experiment is another example of the progress being made toward modern efficient experimentation in the biological sciences.

\* \* \* \* \*

The mathematical model  $Y_i = N(1 - e^{-kX_i})^2$  describing the dose-response relationship for two-break chromosome exchanges had an interesting application to data on the detachment of attached X's in stage-7 oocytes of *Drosophila melanogaster*. Drosophila geneticists agree that if the detachments induced in stage 7 depend on a close pairing relationship of the Y and fourth chromosomes in this stage, an  $N$  value of unity can be predicted. The data from this experiment were fitted by nonlinear least squares to the mathematical model, and the resulting estimate of  $N = 0.946$  was not significantly different from unity. In cases of this type, where the biological material dictates the form that the mathematical model should assume, the correct

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<sup>1</sup>D. A. Gardiner *et al.*, *Ann. Math. Stat.* 30, 1082 (1959).

procedure to follow is one in which the mathematical model is changed to suit the biological model; that is,  $Y_i = (1 - e^{-kx_i})^2$ . Interestingly enough, in this instance, the statistician was not completely apprised of the biological model prior to fitting the two-parameter mathematical model. Only after the numerical results were available, when he suggested to the biologists that the value of  $N$  might, in fact, be unity, did the biologist reason to the correct biological model.

This lesson involving the exchange of information between the biologist and the statistician was very valuable, particularly with this type of nonlinear dose-response model. In general, our experience with fitting nonlinear models has been good. However, one of the most serious shortcomings of our techniques has been our inability to get good estimates of variance for the estimates of the parameters in the model. The variances which we estimate are invariably too high, not because of any shortcoming in the data, but rather because a high linear correlation exists among the estimates of the parameters. Unfortunately, very little is known about this correlation and consequently very little can be done to reduce the estimates of variance. One obvious solution is to have some prior knowledge of the true value of a parameter, and thus to eliminate it as an unknown to be estimated. If one is fortunate enough to have such prior knowledge in a two-parameter model, then estimates of the single remaining unknown parameter, as well as its standard error, can be obtained without difficulty. Such was the case for this problem.

\* \* \* \* \*

In *Drosophila* the expected crossover value,  $P$ , for XXY females is obtained by reducing the observed crossover frequency in XX females by the percent of secondary nondisjunction in XXY females. The value  $P$  is calculated by the formula  $P = B(1 - A)$ , where  $B$  is the total number of crossovers among the male progeny from XX mothers divided by the total number of male progeny (corrected for lethal exceptions) from XX mothers, and  $A$  is twice the number of male exceptions from XXY mothers divided by the total number of male progeny (corrected for lethal exceptions) from XXY mothers. The approximate variance of  $P$  is  $(1 - A)^2 \text{ var}(B) + B^2 \text{ var}(A)$ . For several experiments involving this type of data, the null hypothesis that  $P$  was equal to the observed crossover value for XXY females was tested.

### MAMMALIAN RECOVERY

Analyses have been made of chromosome aberrations induced in the peripheral leukocytes of irradiated humans. The purpose of this study was to provide an opportunity to check *in vitro* observations against material irradiated *in vivo*. The usefulness of the technique as a biological dosimeter depends on the ability to construct calibration curves from actual measurements on irradiated subjects whose physical dose is known.

From information obtained on x-irradiated fresh-drawn human blood, it is possible to make dose estimates from observed aberration rates. Such estimates may be made either from the deletion yield or from the dicentric yield. Since the yield of deletions has been found to be linearly related to dose ( $Y = a + bD$ ) for a given yield,  $Y$ , the dose in rads,  $D$ , may be estimated by the inverse solution  $D = (Y - a)/b$ . Similarly the yield of dicentrics is known to be approximately proportional to the square of the dose ( $Y = cD^2$ ).

Here the inverse solution is  $D = (Y/c)^{1/2}$ . With maximum likelihood estimates of the unknown parameters  $a$ ,  $b$ , and  $c$  calculated from the previously collected laboratory data, it was feasible to estimate, with confidence intervals, the dose required to produce a given number of dicentrics or deletions.

\* \* \* \* \*

Survival of HeLa cells after exposure to  $H^3$ -thymidine exhibits a multitarget dose-response relationship similar to that observed for x-ray killing. The situation here is different, however, in that the irradiation is chronic because tritiated thymidine is stably incorporated into DNA. Since the half-life of  $H^3$  is long compared with the life of a cell, all the descendants of a labeled cell will have a finite, though decreasing, probability of being killed after any number of generations.

The survival probabilities at each generation are conditional on the events of the previous generation. Thus the survival expected in the third generation is higher if both cells in the second generation survive than if only one survives. Since the probability of survival at the fourth generation is almost unity, it is reasonable to consider that the probability of survival of the colony is a function only of the probabilities of survival in the first three generations. A mathematical model describing this dose-response relationship has been constructed and is being tested. Results will be presented in the next annual report.

\* \* \* \* \*

In several studies involving the immunologic antibody-forming cells and homograft reaction in mouse chimeras, and the homotransplantation antigens in mouse hemopoietic tissues, regression analyses were carried out to estimate the functional relationship between antibody response, as measured by titer, and the number of spleen cells transfused. The usual linear least-squares techniques were used to obtain estimates of the regression coefficients, and hypotheses concerning homogeneity of the data and parallelism of the regressions were tested by the standard statistical tests.

\* \* \* \* \*

The survival curve of erythrocytes in guinea pigs was estimated by labeling blood taken from the animals with radioactive chromium ( $Cr^{51}$ ) and injecting the blood in autologous, isologous, or homologous animals. Blood was taken from each animal at seven-day intervals for 70 days, and counts of  $Cr^{51}$  activity were made. A model derived from assumed probabilities of survival was constructed and tested by ten animals in each of the three groups of animals.

Chromium is removed from the blood at a linear rate when a constant number of cells die each day due to senescence. Thus the factor  $1 - k_1 t$  was included in the model to represent this loss, where  $t$  is time in days after injection and  $k_1$  is the constant daily change in the proportion of surviving cells.

Chromium elution is assumed to occur at a rate proportional to the amount of chromium present. In addition, chromium is lost when cells die due to random destruction. These two effects are jointly introduced into the model by the factor  $e^{-k_2 t}$ , where  $k_2$  is the rate of loss due to both causes.

The probability of survival is the product of the two independent factors,

$$P = (1 - k_1 t)e^{-k_2 t}, \quad t \leq \frac{1}{k_1}.$$

Estimates of  $k_1$  and  $k_2$  and standard errors of these estimates were obtained by nonlinear least squares. Thus, survival curves for each group were estimated and hypotheses of differences among the groups were tested.

### RADIATION IMMUNOLOGY

A three-dimensional bioassay experiment was performed using response-surface methodology. The details of the experiment are as follows: To determine the therapeutic value of spleen-cell transplants in irradiated mice, one procedure is to lethally irradiate a group of recipient mice and transplant into them different numbers of spleen cells from unirradiated or sublethally irradiated donor mice. In principle, lethal irradiation of a recipient mouse destroys the therapeutic capacity of all its spleen cells, and in this sense the mouse is comparable to an empty test tube. Then, into such a mouse, one transplants a known number of spleen cells from a donor mouse. If a sufficient number of cells are transplanted, the recipient mouse will survive its lethal dose of radiation. The problem is to estimate the response of lethally irradiated recipient mice, in terms of fraction dying as a function of the number of transfused spleen cells and of the dose of radiation to the donor mice; then, given this function, to determine the relative protective capacity of irradiated spleen cells by considering the relative spleen-cell dose required to give the same response at different radiation doses.

On the basis of previous experimental evidence, the following information was available prior to the experiment (if  $p$  = fraction dying):

1. For a given spleen-cell dose,  $\text{arc sin } \sqrt{p}$  increases linearly with increased radiation dose.
2. For a given radiation dose,  $\text{arc sin } \sqrt{p}$  decreases linearly as the logarithm of the spleen-cell dose increases.
3. The rate of change of  $\text{arc sin } \sqrt{p}$  with respect to radiation dose is constant for all spleen-cell doses in a known range.
4. The rate of change of  $\text{arc sin } \sqrt{p}$  with respect to the logarithm of the spleen-cell dose is constant for all radiation doses in a known range.

This prior knowledge suggested that over a known area of the factor space of radiation dose and the logarithm of the spleen-cell dose, the response, as measured by  $\text{arc sin } \sqrt{p}$ , was the plane:

$$Y = a + bX_1 + cX_2,$$

where  $Y = \text{arc sin } \sqrt{p}$ ,  $X_1 = \log$  spleen-cell dose, and  $X_2 =$  radiation dose. In this instance, the area of the factor space could be described by a parallelogram.

In a square factor space the optimum design for estimating a plane is a factorial design whose treatments are located at the vertices of an equilateral triangle. In such a space the design is orthogonal and the addition of a treatment at the center of the triangle does not destroy the orthogonality. Therefore, the

design which was used was that of an equilateral triangle in a square with a point added at its center to describe a factorial design in four treatments. The triangle was then rotated about its center through a randomly chosen angle. Finally, by a linear transformation, the square was squeezed into a rectangle, and by another transformation the rectangle was twisted into the parallelogram which described the experimental region of the factor space. The coordinates of the four points of the design represented the four points at the factor space at which an experiment would be run. The experimental unit was a group of 25 lethally irradiated mice. Four groups of mice treated according to the specifications of the design constituted one replicate of the experiment and the experiment was performed in two replicates.

The results of the experiment were very satisfactory. For each replicate a plane was fitted and there was no significant difference between the slopes of the planes computed from the two replicates. Thus from a single experiment we could describe the response as a function of two separate independent variables.

To answer the question concerning the relative antibody-forming capacity of the spleen cells, consider a horizontal plane over the area of interest in the factor space and determine the line of intersection with the response plane. If the coordinates of two points on the line of intersection are  $(X_{11}, X_{21})$  and  $(X_{12}, X_{22})$ , the equation of the line of intersection is  $(X_{11} - X_{12}) = k(X_{21} - X_{22})$ , where  $k = c/b$ . But since  $X_1$  is the log of the spleen-cell dose,  $(X_{11} - X_{12})$  is the log of relative spleen-cell dose. Moreover,  $(X_{21} - X_{22})$  represents incremental radiation. Thus, this equation expresses the regression of relative cell dose on incremental radiation. Furthermore, the slope of this line is the ratio of two variables which may be assumed to have the bivariate normal probability distribution. Fieller's theorem provides confidence intervals for this line.

In the experiment a total of eight experimental units in the two replicates, amounting to 200 recipient mice, were used. Normally, an experiment of this type run in the usual manner would involve approximately 1000 recipient mice, which, with considerably more difficulty, would provide similar results.

\* \* \* \* \*

Histologic changes have been observed in the spleen and bone marrow of lethally x-irradiated mice infused with unlabeled spleen and bone marrow in the absence of antigenic stimulation. To determine when, and in what proportion, the donor spleen cells colonize, and what sequence of cellular events they undergo following antigenic stimulation, spleen cells labeled with  $H^3$ -thymidine were followed in heavily irradiated isologous mice in response to sheep red-blood-cell antigens. Using the  $H^3T$  index, namely, the percent labeled cells at a given time divided by the percent labeled cells at the initial time as the response, weighted linear regression analyses were done in which the  $H^3T$  index was fitted against time after treatment. The results of these analyses indicated that the maximum mean-generation time of donor-labeled lymphoidal cells in the recipient spleen can be halved when stimulated by an antigen from about 12 to 24 hr.

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If preimmunized recipient mice react immunologically against the donor, the transferred spleen cells are expected to be totally or partially rejected. In order to obtain a value representing the percentage of rejected donor spleen cells, a study was performed in which the titer in nonsensitized irradiated (B  $\times$  C3H)F recipients was measured as a function of dose of transferred spleen cells. Letting  $Y = \log_2$  titer and  $W = \log_2(cX)$ , where  $X$  = dose of transferred spleen cells and  $c$  is some constant, the regression of  $Y$  on  $W$  was found to be linear, with slope not significantly different from unity. The percentage of rejection, which represents the difference in  $\log_2$  titers between the control and experimental groups, may then be expressed as  $R = [1 - 2^{(Y_E - Y_c)}] 100$ . Approximate confidence limits were evaluated for estimates of  $R$ .

## PATHOLOGY AND PHYSIOLOGY

$I^{131}$ -labeled human serum albumin was used to study protein loss in x-irradiated mice implanted with rat bone marrow. Comparisons were made with normal control mice and with irradiated mice treated with isologous bone marrow. The homogeneity of variances was tested by the variance-ratio test or Bartlett's test, and the hypotheses concerning equality of means were tested using the Student's  $t$  test and the variance-ratio test.

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Irradiation of the mouse early in life causes a displacement of the Gompertz mortality curve, which may indicate induction of precocious senescence. A preliminary study was made on the available mortality data from LAF<sub>1</sub> mice exposed when 6-12 weeks old to gamma rays from an experimental nuclear detonation, RF male mice exposed at 5-10 weeks of age to whole-body x rays, and RF female mice subjected at 10 weeks of age to midlethal doses of whole-body x rays, nitrogen mustard, or triethylene melamine.

The death rates were in some cases computed by the classical actuarial method, and in others by Seal's<sup>2</sup> method. In both LaF<sub>1</sub> and RF mouse strains, the rate of overall mortality tended to increase exponentially with time beyond a certain age, and was displaced upward by radiation and by radiomimetic chemicals. The displacement by radiation was dose-dependent and evident whether mice with or without neoplastic disease were excluded from consideration. Inflections in the curves suggested heterogeneity in the various animal populations. This heterogeneity became more apparent on inspection of mortality with specific diseases.

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<sup>2</sup>H. L. Seal, "The Estimation of Mortality and Other Decremental Probabilities," *Skand. Actuariet.* 37, 137-62 (1954).

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The effect of radiomimetic chemicals on RF female mice was measured in terms of mean-survival time, incidence of leukemia, and incidence of tumors. Two radiomimetic chemicals, nitrogen mustard and triethylene melamine, were used at two and three dose levels respectively, and three separate groups were irradiated with x rays. A control group with no x ray or radiomimetic chemicals was observed. The purpose of the study was to determine whether RF females are affected in the same way by radiomimetic chemicals as they are by x rays. Chi-square tests were performed to see if the data from each agent could be pooled for all doses. Then, where pooling was justified, the hypothesis of equal effects from all agents was tested by chi-square.

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The percentage of mice surviving 30 days after lethal irradiation can be increased by transplantation of bone marrow cells from normal mice or from mice receiving sublethal doses of radiation. Since damaged hematopoietic cells of the recipient are replaced by the injected cells, the number of viable marrow cells injected can be inferred from the percent survival of the recipients. The survival of the recipients is also dependent on physiologic and environmental factors, so that a more direct and accurate method of assessment of marrow-cell growth is desirable. The uptake in the recipient's spleen of a labeled DNA precursor, iododeoxyuridine- $^{131}$ I (IUDR), is such a method.

The statistician and the experimenter cooperated in designing experiments to test the accuracy and reproducibility of the IUDR method. These experiments demonstrated that the method is valid over a hundredfold range of IUDR concentrations, a three- to ten-day range in time elapsed from cell transplantation to IUDR labeling, a twentyfold range of injected cell doses, and up to a radiation dose of 400 r to the donor animals.

A computer program was written to process the experimental data from these experiments and from future experiments which will incorporate the IUDR method. These experiments utilized well-known statistical designs and verified the assumptions required for utilization of a three-dimensional bioassay. Thus, future experiments will be more efficient, as a three-dimensional bioassay using response surface techniques will be employed.

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Experiments were designed to test the effects of different types of bedding on survival of mice. Five types of bedding were used in each of five experiments with three strains of mice. The 20 to 25 pairs of mice used with each bedding in each experiment were housed in separate cages and maintained through five litters. Observations included the number of animals born and the number of survivors at weaning for each pair and for each litter. The analysis consisted of testing hypotheses of differences among beddings as they affect the number born and survival at weaning. Differences among strains and among litters and their interactions with survival were also analyzed.

# Programming Research

## AN ALGORITHM FOR THE SOLUTION OF POLYNOMIAL EQUATIONS BY THE BAIRSTOW METHOD

G. J. Atta

D. C. Ramsey

A. A. Grau

Bairstow's method for the evaluation of the zeros of polynomials is a technique for isolating real quadratic factors of a polynomial with real coefficients. Since every polynomial with real coefficients may be factored into real linear and real quadratic factors, it follows that in theory this method may be used to solve completely any real polynomial equation without resorting to complex computation.

Starting from a trial quadratic factor  $(x^2 + px + q)$ , an improved factor  $x^2 + (p + \delta p)x + (q + \delta q)$  is found as follows. Let  $f(x)$  be a polynomial of degree  $n$ . Two divisions yield

$$f(x) = (x^2 + px + q) g(x) + r_1 x + r_0 ,$$

$$g(x) = (x^2 + px + q) h(x) + s_1 x + s_0 ,$$

where  $r_0$ ,  $r_1$ ,  $s_0$ , and  $s_1$  are functions of  $p$  and  $q$ . It is easily shown<sup>1</sup> that if derivatives of  $r_0$  and  $r_1$  with respect to  $p$  and  $q$  of order higher than the first may be neglected, and if  $(x^2 + px + q)$  has distinct zeros, an improved factor may be obtained by changing  $p$  and  $q$  by amounts determined from  $r_0$ ,  $r_1$ ,  $s_0$ , and  $s_1$ .

Algorithms for the Bairstow process have been in use at ORNL for some time.<sup>2</sup> The latest version written in ALGOL incorporates improvements resulting from the literature and from conversations with J. H. Wilkinson. Garwick's device<sup>3</sup> is used as the convergence criterion. Measures patterned after those of Wilkinson<sup>4</sup> prevent excessive change in step size, which often is accompanied by a serious deterioration in rate of convergence. As in previous algorithms the roots are found in increasing order; however, improvement in the poorly conditioned cases is obtained by using as initial trial factor the one found immediately before.

The algorithm will be tested directly in ALGOL once translators are in use on the IBM 7090 and the CDC 1604. In the meantime, the algorithm has been programmed in IBM FORTRAN using double precision

<sup>1</sup>A. S. Householder, *Principles of Numerical Analysis*, pp 139-41, McGraw-Hill, New York, 1953.

<sup>2</sup>G. J. Atta et al., *Math. Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, p 20.

<sup>3</sup>G. V. Garwick, "The Limit of a Converging Sequence," *Nordisk Tidskrift for Informations Behandling* 1(1), 64 (1961).

<sup>4</sup>J. H. Wilkinson, "The Evaluation of the Zeros of Ill-Conditioned Polynomials. Parts I and II," *Numerische Math.* 1, 150-80 (1959).

arithmetic. Excellent results have been obtained from this on such things as the ill-conditioned polynomial used as an example by Olver.<sup>5</sup> The results are in agreement with (although not as accurate as) those obtained by Wilkinson's<sup>4</sup> use of the same polynomial.

### THE CONTROL DATA CORPORATION 1604 ALGOL COMPILER

L. L. Bumgarner

A. A. Grau

R. G. Stueland<sup>6</sup>

K. A. Wolf<sup>6</sup>

The cooperative project<sup>7</sup> undertaken with Control Data Corporation to construct an ALGOL compiler for the CDC 1604 computer is nearing completion in development and entering the field-test stage.

#### General Characteristics

The compiler makes two passes on the ALGOL source program. During the first pass, the symbols are converted to an internal format of one computer word for each identifier or delimiter, and a check is made on the following types of errors: (1) syntactical errors, (2) misspelled delimiters, (3) missing escape symbols, and (4) incomplete, inconsistent, and redundant declarations. Some errors can be corrected; others cannot, and a message will appear on the listing of the source program to indicate each of these. In the latter case, no translation is attempted. Otherwise, the second pass will be made to effect translation. The original plan of adapting the IBM 7090 SHARE syntax checker to the CDC 1604 did not prove entirely workable, and although some ideas were borrowed from that program, the two passes possess much of the same general structure.

#### Control System

A control program was written to integrate the compiler into the CO-OP Monitor Programming System. This program provides for the option of direct machine code compilation or the intermediate use of assembly language. The latter is useful for mixing with other languages and for compiling procedures separately from a calling program. This kind of flexibility is not completely attainable within the framework of ALGOL, and a new type of declaration must be introduced. The declarator **external** was added to enable the compiler to link separately compiled procedures (whether library routines or not) and assembly language subroutines to an ALGOL calling program. Each such procedure or subroutine must be declared **external** in the ALGOL program. This declarator will be preceded by a type declarator in the case of a function; an example of such a declaration is

**real external** Bessel, Gamma.

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<sup>5</sup>F. W. J. Olver, "Evaluation of Zeros of High Degree Polynomials," *Phil. Trans. Roy. Soc. London, Ser. A*, 244(885), 385-415 (1952).

<sup>6</sup>Cooperative programmers from Control Data Corporation.

<sup>7</sup>*Math. Panel Ann. Progr. Rept. Dec. 31, 1961*, ORNL-3264, pp 8-9.

### Language Restrictions

The language restrictions imposed are near those anticipated.<sup>7</sup> The restriction that quantities must be declared before use has been lifted, but the call of arrays by value has not yet been incorporated. The restrictions on type are the following:

1. The exponentiation operation is redefined to prevent the type of an expression from depending upon the value of an exponent: the expression  $x \uparrow y$  will be of type **real** unless  $x$  is of type **integer** and  $y$  is a nonnegative integer constant.
2. The simple arithmetic expressions occurring as constituents of conditional arithmetic expressions must be of the same type.
3. The arithmetic type of an actual parameter must be the same as that of the corresponding formal parameter, the type of the latter assumed to be **real** unless specified.

### Input-Output

The input-output facilities use three reserved names: *input*, *output*, and *read*. *Input* and *output* cause activation of the standard FORTRAN routines. They were made somewhat more flexible by the introduction of two new declarators: **format** and **list**. The declarator **format** associates an identifier with a format string, as in the following example:

```
format F := '(10X, 3E20.7)' .
```

Any FORTRAN format is allowed. The declarator **list** names a list of expressions, and **for** clauses can be used for grouping array elements, as for example:

```
list L := a, x + y, if B then u else n + 2,  
for i := 1 step 1 until m do T[i] .
```

The use of these declarators, while in many cases convenient, is not necessary. The *input* and *output* routines can have any number of parameters, and the following two output statements are equivalent, with *F* and *L* as declared above:

```
output (51, F, L)  
output (51, '(10X, 3E20.7)', a, x + y, if B  
then u else n + 2, for i := 1 step 1  
until m do T[i]).
```

The *read* routine is not associated with the FORTRAN mechanism. It inputs numbers in any ALGOL form, written free field, making any type conversions necessary. It reads only from the standard input medium. There may be any number of parameters, as for example:

```
read (S, t, x[n]) .
```

The intermediate tape-handling facilities are not complete, but they will also make use of available FORTRAN routines.

### Compiler Size and Tables

The compiler occupies approximately 6100 words of instructions. The tables are not of fixed length. Initially, each table is allocated one word. When more space becomes necessary for a table, five more words are allocated by moving all the tables in lower address locations than the given table. This maneuver is repeated each time any table needs more space. The output from the first pass is also given space in core memory until it and the tables consume all available space. If this happens, all of the output is written on magnetic tape to make more room for both tables and output. This will be done as many times as necessary. If any output has been written on tape, at the end of the first pass the rest of the output is also written on the tape, and all of this information is buffered back into memory as the second pass is made. If for any identifier the full information was unavailable at the time that this location was written on tape, a request entry is made in a special table to indicate that this information is to be filled in when the location is brought back into memory.

### SHARE ALGOL PROJECT: ALGOL 60 PROCESSOR FOR THE IBM 709/7090

Marjorie P. Lietzke      A. A. Grau

A syntax checker was designed based on the syntax of ALGOL, described in the ALGOL 60 report.<sup>8</sup> This syntax checker was described briefly in ORNL-3264<sup>9</sup> and in detail in ORNL-3399.<sup>10</sup> Since the definition of the elements of the language is recursive, it was found most desirable to design the syntax checker as a set of mutually recursive processors tied together by building blocks which perform certain bookkeeping functions. Because of the recursive nature of the language and of the syntax checker the problem of recovery after an error required much attention. A method was devised which permits most programs to be checked completely despite errors. The syntax checker has been implemented for the IBM 7090 as a part of the SHARE ALGOL processor and has operated very satisfactorily.

Since March 1961, the processor has been converted from the SOS system to the FAP-FORTRAN system and is almost ready for general distribution. The number of IBM installations taking an active interest in the ALGOL project has increased from a low of four in September 1960 to over 30 at present.

The processor has been used for production work for several ORNL problems and has given very satisfactory results.

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<sup>8</sup>J. W. Backus *et al.*, *Communs. Assoc. Comput. Mach.* **3**, 299-314 (1960).

<sup>9</sup>*Math. Panel Ann. Progr. Rept. Dec. 31, 1961*, ORNL-3264, p 7.

<sup>10</sup>Marjorie P. Lietzke, *An ALGOL Syntax Checker for the IBM 7090 Computer*, ORNL-3399 (in press).

## DESIGN OF ALGOL INPUT-OUTPUT

L. L. Bumgarner

Manuel Feliciano

A. A. Grau

ALGOL 60 contains no specifications for input-output facilities; it simply allows for the possibility of procedures expressed in non-ALGOL code. To retain the machine independence of the language and facilitate program exchange, it is desirable that those constructing ALGOL compilers agree on the design of the input-output procedures. This is made difficult by the large variations in input-output hardware, particularly between large and small computers.

Discussions were undertaken with other members of the ALCOR group to design an input-output system suitable for large-scale computers utilizing line printers. Many of the present ALGOL compilers, including that for the Control Data Corporation 1604, make use of existing FORTRAN input-output routines. These routines have characteristics undesirable for use with ALGOL, and in order to make satisfactory use of them it is necessary to make *ad hoc* additions to the ALGOL language. In the work with ALCOR, effort was made to keep the input-output system within the framework of ALGOL without sacrificing any of the versatility available with the FORTRAN system.

At present the discussions have resulted in several fruitful ideas and substantial areas of agreement. As the system would look to the programmer, there are a number of reserved-name procedure identifiers such as *format*, *space*, *margin*, *line*, *page*, *print*, and *read*, and a declarator *string*. The latter is the sole addition to the language and simply extends the existing specifier *string* to the role of declarator. As can be inferred from the names of the above procedures, several control the line printer. The following features of the system are notable:

1. The format of numbers is established by a procedure call. This format remains active until replaced by another such procedure call.
2. A free format is allowed. This is established by a call of *format* with an empty format string. Under input this means that numbers of any legal form are accepted. Under output it yields numbers in scientific notation if declared *real* and as integers if declared *integer*.
3. The format string in a call of *format* is a number the form of which is that of the numbers being read or printed. For example, '00.0000' means the number is to have 2 places before and 4 places after the decimal point.
4. For output, a buffer region is established, with its length given by a call of *margin*, such as

*margin* (10,80) .

This establishes on the printer an indentation of 10 spaces on the left and a right margin so that 71 characters can be printed. At a call of *print*, the numbers to be printed are properly converted and stored in the buffer region sequentially from left to right. As long as space remains in the buffer, this is continued. When the buffer region is full, the line is put out and the buffer is reset for the next line. This process is interrupted by a call of *line* or *page*, calling for a new line or new page, respectively, as anything in the buffer will be put out at this point.

# Programming and Analysis

## ANALYTICAL CHEMISTRY AND CHEMICAL TECHNOLOGY

H. P. Carter      D. A. Gardiner      D. C. Ramsey

### Cask-Drop Experiments

During cask-drop experiments strain gage data are obtained by recording charts. From these data, which vary with the gage factor, a maximum deformation and a permanent deformation can be computed. A computer program was written to fit a curve to known deflections caused by known resistances. With this curve the deflections produced by the drop were used to compute the deformations. Both linear and cubic curve fits were used.

### Gas Composition

A program was written for calculating the weighted average composition, in volume percent and moles per gram of carbide, of complex mixtures of gaseous hydrocarbons, based on the areas under the peaks in the gas chromatograms, calibration constants for the instrument, sample volumes, and total moles of gas. This program has been used routinely to calculate the composition of 40 component hydrocarbon mixtures produced in the reactions of uranium and thorium carbides with water and nonoxidizing acids and bases such as HCl, H<sub>2</sub>SO<sub>4</sub>, and NaOH. The program will handle multiple samples, showing both the composition of each sample and the average composition of all gas produced in the experiment. It is a flexible program and could, with minor modifications, be used to calculate the composition of any gas mixture which can be analyzed by gas chromatography.

### Time and Cost Distributions

Two computer programs have been written for the Analytical Chemistry Division to produce their monthly time and cost distribution reports.

For each laboratory within the division the first code prepares a report of the percentage of time spent on each customer account. Within each laboratory report the accounts are ordered and reported according to customer divisions. This information in its ordered form is stored on magnetic tape to be used by the second program.

Once the monthly cost of operation for the Analytical Chemistry Division has been determined, the second code uses this information to compute a cost for each of the accounts. Again a report for each laboratory is given. In addition to these a report for each customer division is produced, showing all work done by each laboratory for the customer division.

#### Calibration of a Carbon Content Analyzer

Previous practice in calibrating a carbon content analyzer has been to use seven distinct values of carbon content to determine the linear calibration equation. It appeared, however, that more precise results could be obtained from a system requiring the use of only four distinct carbon values. The statistical problem was to recommend a design that would do at least as well as the current system in determining the slope coefficient. In doing this, the conservative assumption was made that the experimental error for the proposed system was equal to the experimental error for the seven-point system, and the approximation due to Harris, Horvitz, and Mood<sup>1</sup> was applied.

This required the collection of four sets of data at each of the four carbon points on each of three days. (Three sets on each of four days would be equally good.) With this design the investigator could obtain, with 95% assurance, a 95% confidence interval which is no wider than those determined in the past.

#### The SADSAC Device

A  $4^2$  factorial design in four replications was recommended to study the variability in an instrument named the Semi-Automatic Device for Spectrographic Analog Computation (SADSAC). The contrived input for this 16-channel device consisted of the  $4^2$  combinations of four levels of intercept and four levels of time. These combinations were run twice a day for two days on each of the 16 channels.

Estimates of variability were calculated for each channel separately by means of the analysis of variance. In addition, the expected values for each of the  $4^2$  combinations were computed according to theory, and the ratios of the observed response to the expected response were analyzed by the analysis-of-variance technique. The ratios are estimates of bias; hence the analysis was capable of labeling the source and estimating the amount of such bias.

**Electrode Systems.** — A project to evaluate many different electrode systems for use in spectrographic analysis was begun during this report period. By using the SADSAC, up to 16 different chemical elements could be measured by a single electrode system. A simple random design was sufficient for obtaining the appropriate data. Currently, this design in ten replicates has been used to evaluate 16 different electrode systems.

Two statistical analyses are applied to the data for each electrode system. One analysis examines the variation among replicates for each chemical element individually, applying Bartlett's test of homogeneity to the estimated "within elements" mean square. No lack of homogeneity has been discovered so far.

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<sup>1</sup>Marilyn Harris, D. G. Horvitz, and A. M. Mood, *J. Am. Stat. Assoc.* 43, 391-401 (1948).

The data are also analyzed by the analysis-of-variance technique. From this analysis the "elements by replications interaction" mean square is taken as the estimate of experimental variance. The better electrode systems are those with the smaller experimental variances.

### Report of Analysis

A program has been written to compute the results of chemical analyses and to produce a customer report for one of the Analytical Chemistry laboratories. As input the program uses the measurements recorded by laboratory technicians during analysis. These measurements are recorded by the technician on sheets from which the input can be typed directly.

## CHEMISTRY

G. J. Atta      K. O. Martin

### Crystallography

The following programs have been prepared and put into general use:

1. A FORTRAN general linearized least-squares adjustment of many parameters (ORGLS).<sup>2</sup> This program requires a user's subroutine for the function to be fitted and its derivatives; optionally, the derivatives may be computed by numerical differentiation.
2. A FORTRAN program for least-squares adjustment of the parameters of crystal structures (ORFLS).<sup>3</sup> This is a specialization of ORGLS to the specific computations involved in the determination of atomic arrangements in crystals. This program parallels an older IBM 704 version written in SAP language (ORXLS).<sup>4</sup>
3. A FORTRAN program to process the results of crystal-structure determinations (ORFFE). This program computes a variety of derived functions of the basic crystal-structure parameters and the associated standard errors, and gives the results of the least-squares refinement as the output of ORFLS. Examples are interatomic distances and bond angles. This is based on an older IBM 704 program which was partially in SAP language (ORXFE).<sup>5</sup>
4. A program to process data collected by the Oak Ridge Automatic Neutron Diffractometer, written partly in FORTRAN and partly in machine language, replacing an older Oracle program.
5. A program to produce instruction paper tapes for the Oak Ridge Automatic Neutron Diffractometer, replacing an older Oracle program.

<sup>2</sup>W. R. Busing and H. A. Levy, *OR GLS, A General Fortran Least Squares Program*, ORNL TM-271 (Aug 7, 1962).

<sup>3</sup>W. R. Busing, K. O. Martin, and H. A. Levy, *OR FLS, A Fortran Crystallographic Least-Squares Program*, ORNL TM-305 (Nov. 21, 1962).

<sup>4</sup>W. R. Busing and H. A. Levy, *A Crystallographic Least Squares Refinement Program for the IBM 704*, ORNL CF-59-4-37 (May 4, 1959).

<sup>5</sup>W. R. Busing and H. A. Levy, *A Crystallographic Function and Error Program for the IBM 704*, ORNL CF-59-12-3 (Dec. 9, 1959).

### Miscellaneous

The curve  $C = C_0 e^{-kt}$  was fitted to some chemical concentration data to obtain least-squares estimates of  $C_0$  and  $k$ .

The curve  $Y = T_2(1 + D_{23}K_{23} + D_{24}K_{24})$  was fitted to some raw data to obtain least-squares estimates of  $T_2$ ,  $K_{23}$ , and  $K_{24}$ .

### HEALTH PHYSICS

G. J. Atta	D. G. Gosslee
H. P. Carter	M. T. Harkrider
Arline H. Culkowski	R. P. Leinius
D. A. Gardiner	D. C. Ramsey

#### Analysis of Sr<sup>90</sup> Excretion-Rate Data

Four models for Sr<sup>90</sup> excretion-rate data were investigated. The models considered were (1)  $E = At^{-B}$ , (2)  $E = A(1 + Ct)^B$ , (3)  $E = Ae^{-\alpha t} + Be^{-\beta t} + Ce^{-\gamma t}$ , and (4)  $E = Ae^{-\alpha t} + Be^{-\beta t} + Ce^{-\gamma t} + De^{-\delta t}$ .

Nonlinear least-squares methods yielded estimates of  $A$ ,  $B$ ,  $C$ , and their standard errors for cases 1 and 2. Convergence of the iterative process was not achieved in cases 3 and 4.

#### Urinalysis Data on Plutonium

The data on terminal hospital patients injected with Pu<sup>239</sup> were reported at 24-hr intervals. If the fraction of a single dose injected into the blood excreted per unit time at time  $t$  is taken to be a power function  $at^{-\alpha}$ , the fraction of the injected dose excreted on the  $i$ th day is

$$F = \int_{i-1}^i at^{-\alpha} dt = \frac{a}{1-\alpha} [i^{1-\alpha} - (i-1)^{1-\alpha}].$$

Urinalysis data for this model were fitted by nonlinear least-squares techniques to estimate the constants  $a$  and  $\alpha$ .

#### Electron Time-of-Flight Measurements of Diffusion and Drift Velocity

Consider the motion of a packet of electrons which at time  $t = 0$  is spread uniformly over a plane normal to the  $x$  direction at  $x = 0$ . Assume that the electrons are diffusing with coefficient  $D$ , are drifting in the  $x$  direction with velocity  $w$ , and are captured at a rate  $w\beta$ . If the electric field of strength  $E$  (v/cm) is imposed in the  $x$  direction in a gas at pressure  $P$ , then the differential equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} - w \frac{\partial n}{\partial x} - \beta w n$$

gives the volume density,  $n$ , of electrons as a function of  $x$  and  $t$  provided the diffusion equation can be restricted to one spatial dimension. A solution to the differential equation for a source which has an area density  $N$  over the  $x = 0$  plane at  $t = 0$  is

$$n(x, t) = Awt^{-1/2}e^{-(x-wt)^2/4Dt}e^{-\beta wt},$$

where  $A = N(4\pi D)^{-1/2}$ .

Electron-swarm experiments may be arranged to satisfy the boundary conditions applicable to the one-dimensional, time-dependent, diffusion-drift equation. If a detector that is capable of resolving individual electrons is placed at a point on a plane which is  $L$  cm from another plane releasing electrons at time  $t = 0$ , then a measurement of  $n(L, t)$  would provide, by least-squares curve fitting, estimates of the four quantities  $N$ ,  $D$ ,  $w$ , and  $\beta$ .

Results for  $N$ ,  $D$ ,  $w$ , and  $\beta$  have been obtained for a few gases, but they have varied from the results of other investigators. It is conjectured that these discrepancies are due to inaccuracies in the time-calibration curves. Methods to determine time curves more precisely are under way.

### Ecology

**Regression Analyses on Inflorescence of Local Sedges.** — The sedges, *Carex frankii* and *Carex vulpinoidea*, which grow in abundance in the Oak Ridge area, furnish some interesting information about the effect of radiation on inflorescence. Investigators in the Health Physics Division collected data on the length of the flowering stems of the two sedges from plants growing naturally in the bed of White Oak Lake and the surrounding area. Each plant of those measured belonged to one of seven sets, which differed according to the constituents of the soil and the amount of radiation to which the plant was subjected. Inflorescence was measured on 50 plants in each set. In the absence of a theoretical model to relate the length of stem to radiation and soil constituents, regression analyses are being performed to suggest a model.

Statistical "experimentation" might be viewed as a by-product of this investigation. With the aid of computer programs distributed by the University of California at Los Angeles, a great number of linear models are being tried. Through this effort we are gaining some insight into the result of applying a dubious but widespread method known as step-wise regression analysis.

**Leaf Decomposition.** — The analysis of factors affecting the decomposition of leaves was continued.<sup>6</sup> Data additional to the fungal and bacterial counts became available and were punched on cards.

Leaves from four species of trees were stored in bags under three different species of forest stands. Samples were taken from the bags at two-week intervals, and observations on bacterial and fungal counts, mycelium growth, weight loss,  $\text{CO}_2$  loss, and moisture content were made. Further tests of hypotheses

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<sup>6</sup>Math. Panel Ann. Progr. Rept. Dec. 31, 1961, ORNL-3264, p 25.

of differences in the observations among species and stands were made by analyses of variance. Regression analyses to test models relating the observed variables have been initiated. The regression analyses will be continued, to construct a model which will best describe the relationship among the observed variables.

#### Whole-Body Counting

During this report period preliminary investigations into whole-body counting of persons working in and residing near an atomic energy establishment were begun. Questionnaires designed to elicit information on eating habits of ORGDP personnel were distributed by ORGDP management. From these, information on length of employment, amounts of milk and water drunk, and amounts of green vegetables, bread, and locally caught fish eaten was obtained and transferred to punched cards. The Health Physics Division is now using this information to select individuals for whole-body counting.

#### Cell-Size Distribution

Measurements of the sizes of white and red blood cells can be made by a Coulter counter. Records from the instrument indicate the frequency of cells of various sizes. Estimates of the mean cell size and the total volume of cells can be obtained easily from this frequency distribution when the record does not contain counts of other types of cells and when the frequency distribution is sufficiently far removed from "noise" at the lower end of the scale. However, when either of these interferences is present the counts for some cell sizes include counts in addition to counts of the cell type of interest.

An approximate procedure has been developed for estimating the mean cell size and the total cell volume when the degree of overlap of the distribution of counts of interest with the distribution of counts from interference is moderate. The cell sizes are transformed to logarithms in order to make the frequency distribution approximately normal.<sup>7</sup> A point of truncation is estimated that will exclude the counts due to the interference. Then a method for estimating the mean and variance for singly truncated normal distribution is employed.<sup>8</sup> Finally, an estimate of the total volume of cells and its variance is calculated from the mean and variance of the distribution of cell sizes.

#### White Oak Lake Bed Studies

The sample survey plan for the White Oak Lake bed reported in the last annual report<sup>9</sup> was revised to incorporate additional information on the radioactivity of the bed as obtained from samples arbitrarily chosen in 1962. In accordance with the new plan, 250 two-foot cores of the lake bed soil have been removed and the soils are being analyzed. Analysis of all the soil samples will provide estimates of the total amount of radioactivity in the White Oak Lake bed.

<sup>7</sup>George Brecher *et al.*, *Ann. N. Y. Acad. Sci.* **99**, 242 (1962).

<sup>8</sup>A. C. Cohen, *Technometrics* **1**, 217 (1959).

<sup>9</sup>Nancy B. Alexander *et al.*, *Math. Panel Ann. Progr. Rept. Dec. 31, 1961*, ORNL-3264, p 26.

### Secondary-Electron Cascades in Metals

The processes by which electrons with energies of the order of tens to hundreds of electron volts lose their energy in metals are of considerable interest in connection with secondary-electron emission, and in connection with the comparison of observed and calculated electron energy distributions in media containing radioactive sources. Interaction cross sections for electrons in a degenerate free electron gas have been used in order to approximate cross sections for conduction-band electrons in real metals. The pertinent cross sections are those appropriate to (1) single particle excitations and (2) the excitation of plasma oscillations in the free electron gas. These cross sections have been computed and used in a numerical solution of the slowing down and cascade spectra resulting from electrons which are low enough in energy that interband transitions are not possible. These spectra, corrected for reflection at the surfaces, will be compared with experimental data on secondary-electron energy distributions from metals.

### Programs Related to O5R

The code for study of sodium activation by neutrons incident on a "phantom" body, which was previously written for the IBM 704, has been recoded for use on the IBM 7090.

The O5R program was used to create a history of neutrons incident, in a beam, on a human head. A routine was then written to analyze these histories in connection with medical research on irradiating tumors in the head. More work will be done in this area when more accurate values for the composition (hydrogen, oxygen, etc.) of the human head are available.

The codes for analysis of collision histories written by O5R for a cylinder geometry have been written for the IBM 7090. These include analysis for collision densities and energy deposition. Previously, these codes were written for use on the IBM 704 for slab geometry.

### Portable-Instrument Service Data

In order to study portable-instrument service data more effectively, a computer program was written. The program sorts and reports the instruments along with pertinent service information over a given period (1) according to instrument type, (2) according to X number, and (3) according to area offices. The program also lists those instruments whose service data meet certain conditions which warrant special attention. These instruments are reported (1) according to instrument type and (2) according to X number.

### INFORMATION RETRIEVAL

Nancy B. Alexander

Library

The Technical Information Division and the Mathematics Division are producing Key Word Indices, using a program written for Bell Telephone Laboratories. The input of this program consists of cards containing titles, authors, document numbers, cross references, and other pertinent information. The

code compares each word of each title with an internally stored list of nonsignificant words. The title or a portion of it is listed for each appearance of a significant word. The complete list is printed out with all significant words vertically aligned in alphabetical order. In addition, a bibliography is produced and cards containing author and document number are punched. These cards are sorted to produce an alphabetized author index. Temporary changes to the nonsignificant word list may be made for all or parts of any computer run.

The program is set up to run in the local IBM 7090 monitor system and has been used to produce monthly, semiannual, and annual indices to the titles of the reports issued by the Laboratory and received in the Document Collection Section of the Central Research Library, and an index to a division annual progress report. The internal nonsignificant word storage was modified, the maximum entry length was increased to accommodate short abstracts in addition to titles, and the output format was altered to fit certain local requirements.

This program will be used to produce indices for monthly reports on documents generated by the Laboratory, for annual progress reports, and for personal and division document files.

## INSPECTION ENGINEERING

D. A. Gardiner

### Filter Tests

Inspection engineers at ORNL are required to test a large number of high-efficiency filters and to report the efficiencies of these filters. Their report is a form of certification and, of course, they wish to assert the confidence with which they certify the filters.

In order to estimate the variability in the inspection process, an experimental design involving two filters was prescribed. One filter was randomly selected from an apparently good stock. The other was a filter which, by visual examination, was seen to be damaged. Each of five inspectors inspected each filter five times independently on a photometer using a 90% concentration of smoke and then repeated the process with a 50% concentration of smoke.

From this experiment the magnitudes and sources of variability may be determined. When subjected to an analysis of variance, the data will provide mean squares of which appropriate linear combinations may be constructed to provide estimates of variability for certification statements.

## METALS AND CERAMICS

Nancy B. Alexander	Barbara A. Flores
G. J. Atta	D. A. Gardiner
H. P. Carter	M. M. Goff
Arline H. Culkowski	Jeuel G. LaTorre
M. Feliciano	C. W. Nestor, Jr.

### Alloy Calculations for Delta-Function Atoms

A portion of this calculation involves the solution to the pair of transcendental equations

$$\begin{aligned} \cos x \cosh y - \alpha, \\ \sin x \sinh y = \beta; \end{aligned} \quad (1)$$

that is, to find the complex number  $P = x + iy$  such that

$$\cos P = \alpha - i\beta,$$

subject to the restrictions that  $0 \leq x \leq \pi$  and that  $y < 0$ . A FORTRAN subroutine was programmed to solve the pair of equations (1) using the direct-search procedure of Hooke and Jeeves.<sup>10</sup> The quantity  $Q$  is defined as

$$Q \equiv |\cos x \cosh y - \alpha| + |\sin x \sinh y - \beta|,$$

and  $x$  and  $y$  are changed in small uniform steps until no further reduction in  $Q$  can be made. If a preset number of step-size reductions have been made, the calculation is finished; if not, the step size is reduced and more searching is carried out. Since the step size is uniform, the addition formulas for trigonometric and hyperbolic functions are used to compute the necessary functions during the search with a particular step size. In this way explicit calculation of trigonometric and hyperbolic functions is necessary only when the step size is reduced. In a test case the subroutine was used to evaluate 300 solutions of Eqs. (1); this was done in 1 min of computer time, using six step-size reductions. The largest  $Q$  value was  $5 \times 10^{-7}$ ; most were of the order of  $10^{-8}$ .

### Evaluation of Fiber Textures for Cubic Metals

Fiber textures can be represented in two ways:

1. As distribution of different crystalline axes with respect to the physically distinguished axis (fiber axis)
2. As distribution of the fiber axis in the crystal lattice

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<sup>10</sup>Robert Hooke and T. A. Jeeves, "'Direct Search' Solution of Numerical and Statistical Problems," *J. Assoc. Comput. Mach.* **8**, 212 (April 1961).

The second representation, being a superposition of all possible distribution of the first kind, gives much more information. It cannot, however, be obtained experimentally in a direct way.<sup>11,12</sup>

The experimental information, gained by x-ray analysis, is the distribution  $I(\psi)$  of the normal of a particular family of crystal axes  $\{hkl\}$  as a function of the angle  $\psi$  between this crystal axis and the fiber axis, averaged over the azimuth  $\beta$  around the fiber axis (representation 1). This is the same as the average over the azimuth  $\alpha$  around the crystal axis  $\{hkl\}$  of the distribution  $T(\phi\alpha)$  according to representation 2 ( $\phi, \alpha$  are polar coordinates in the lattice,  $\{hkl\}$  being the polar axis). Thus we can write:

$$I(\phi) = \frac{I_0}{2\pi} \int_0^{2\pi} T(\phi, \alpha) d\alpha, \quad (1)$$

in which

$$I_0 = \int_0^{\pi/2} I(\phi) \sin \phi d\phi,$$

the factor  $I_0/2\pi$  being introduced for normalization.

The problem is now to find  $T(\phi, \alpha)$  when  $I(\phi)$  is given for a few crystal axes (usually  $\{001\}$ ,  $\{011\}$ ,  $\{111\}$ ).

As Bunge<sup>13</sup> has shown, this problem can be handled by taking into account the symmetry of the crystal. For cubic symmetry  $T(\phi, \alpha)$  can be expanded in a series of cubic harmonics:

$$T(\phi, \alpha) = \sum_m K_m S_m(\phi, \alpha), \quad (2)$$

where

$$S_m(\phi, \alpha) = \sum_{k=0}^{M/c} S_m^k(\phi) \cos k\alpha, \quad (3)$$

in which  $c$  is a constant, dependent on the symmetry of the polar axis. For  $\{001\}$ ,  $c = 4$ ; for  $\{111\}$ ,  $c = 3$ ; for  $\{011\}$ ,  $c = 2$ . If we set this into Eq. (1) we obtain:

$$\begin{aligned} I(\phi) &= \frac{I_0}{2\pi} \int_0^{2\pi} \sum_m K_m \sum_{k=0}^{M/c} S_m^k(\phi) \cos k\alpha d\alpha \\ &= I_0 \sum_m K_m S_m^0(\phi). \end{aligned} \quad (4)$$

<sup>11</sup>L. K. Jetter, C. J. McHargue, and R. O. Williams, *J. Appl. Phys.* **27**, 368 (1956).

<sup>12</sup>G. V. Czjzek, *Met. and Cer. Div. Ann. Progr. Rept. May 31, 1962*, ORNL-3313, p 190.

<sup>13</sup>H. J. Bunge, *Monatsber. Deut. Akad. Wiss. Berlin* **1**(1959) 400.

The problem is now reduced to the determination of the coefficients  $K_m$ . The easiest method, to construct the system of functions  $S_m(\phi, \alpha)$  such that the  $S_m^0(\phi)$  form a complete, orthonormal system, is not applicable because there are more functions needed in two dimensions than in one dimension. It is, however, possible to make all  $S_m^0(\phi)$  orthogonal to each other. Then for certain  $m$ ,  $S_m^0(\phi) = 0$  and the corresponding  $K_m$  do not appear in Eq. (4). These "missing" coefficients can be calculated by going through the procedure for several crystal axes. There are linear relations between the functions  $S_m(\phi, \alpha)$  for different axes, which are used to set up a system of linear equations for the "missing" coefficients  $K_m$ .

A program is being written to determine  $T(\phi, \alpha)$  for given  $I(\phi)$ , using a system of 34 functions for each of the poles {001}, {011}, and {111}.

### High-Flux Isotope Reactor Fuel Plates

Statistical problems presently arise in the HFIR project at three distinct stages of the manufacture of the fuel plates. Analysis of preliminary information gathered on the powder metallurgy process of fabricating fuel plate cores is now in progress. Hence at the first stage a plan for obtaining core-height measurements was developed, and adopted by the metallurgists, and data from several randomly selected cores are in hand. These data will provide valuable information on the variability of the fuel profile within the cores. Also, from these data the core fabricators will gain insight into how best to press the powders to meet the reactor specifications.

The second stage of the project in which statistical problems arise is the stage of rolling the metals into the fuel-plate form. A design for sampling within the fuel plate was carried out and tolerance limits for fuel concentrations were calculated. The data for this part of the study were derived from chemical analyses of sections punched from the fuel plates according to a factorial plan.

The fuel element for HFIR will be replaced approximately every two weeks. Therefore, at this third stage, a practical method of inspecting the hundreds of fuel plates before assembly into the fuel element must be worked out. Discussions are under way with personnel of the Nondestructive Testing group of the Metals and Ceramics Division to devise means of accomplishing this task.

### Thorium Oxide Pellets

The analysis of the hot-pressed densities of thorium oxide pellets as obtained from the experimental design described in last year's report<sup>14</sup> was completed. A report of the results has been published by the metallurgists in charge.<sup>15</sup>

The experiment was performed using a three-dimensional central composite design of the type useful for investigating second-order response surfaces. The response contours were approximated by the method of least squares, and a three-dimensional plastic model was constructed to illustrate the results.

<sup>14</sup>Arline H. Culkowski *et al.*, *Math. Panel Ann. Progr. Rept.* Dec. 31, 1961, ORNL-3264, p 32.

<sup>15</sup>C. S. Morgan and C. S. Yust, *Met. and Cer. Div. Ann. Progr. Rept.* May 31, 1962, ORNL-3313, pp. 141-43.

### Uranium-Aluminum Alloys

The analysis of the data obtained from the experiment on hardness of uranium-aluminum alloys as described in the previous annual report<sup>16</sup> was accomplished. In this experiment, hardness as a function of annealing time, annealing temperature, and cold reduction was approximated by a second-order polynomial for each of three alloys.

In all three cases the independent variables were statistically significant contributors to the function in both their linear and quadratic representations. However, for one alloy there still remained a significant amount of variation which could not be accounted for by the model.

### Analysis of Fused-Salt Absorption Spectra

A program was written for the IBM 7090 to reduce data from measurements of the absorption spectra of fused salts, and to obtain the parameters of an assumed form for the reduced spectral profiles by a nonlinear least-squares procedure. Revisions to an earlier program for the Oracle<sup>17</sup> include the use of magnetic-tape input, replacement of the sections using the Oracle and Moseley curve plotters with a section using the Calcomp plotter, the use of a modified Gauss-Newton method<sup>18</sup> to speed convergence to the nonlinear least-squares procedure, and various additions to the output.

### Resistance-Thermometer Table

An IBM 7090 FORTRAN program was written to compute a table of resistances for a low-temperature thermometer.

### NEUTRON PHYSICS

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### Calculation of Pair-Production Cross Sections

Preliminary work was begun during the period on the construction of a program designed to calculate differential energy and angular cross sections for each member of a pair of Dirac particles produced by an unpolarized photon. For each incident photon energy a particular distribution of the available kinetic energy between the pair of particles must be selected. The program is then to calculate the coefficients

<sup>16</sup>Arline H. Culkowski *et al.*, *Math. Panel Ann. Progr. Rept.* Dec. 31, 1961, ORNL-3264, p 32.

<sup>17</sup>*Math. Panel Ann. Progr. Rept.* Mar. 1, 1957 to Aug. 31, 1958, ORNL-2652, pp 27-28.

<sup>18</sup>H. O. Hartley, "The Modified Gauss-Newton Method for the Fitting of Non-Linear Regression Functions of Least Squares," *Technometrics* 3, 269-80 (May 1961).

of the Legendre polynomial expansion of the angular distribution of each particle (electron and positron) independent of the direction of the other. The maximum order polynomial in the expansion is to be an input number to the program.

A rather extensive set of subroutines is needed for this program, including one for the calculation of the hypergeometric function of two independent real variables with complex parameters, one for the calculation of the real part of the gamma function of complex argument, and one for the calculation of Clebsch-Gordan coefficients. Effort to date on this problem has been concentrated on locating existing FORTRAN subroutines (if any) and on programming a FORTRAN subroutine for the hypergeometric function calculation.

### The O5R Code

An addition was made to O5R in order to allow inelastic scattering and  $(n,2n)$  reactions to be taken into account. The general geometry routine, GEOM, was incorporated into the code in order to handle any reasonable configuration of material media. The IBM 7090 FAP version was completely rewritten in the FORTRAN language and partially checked out on the 7090. An addition is being checked out to allow anisotropic scattering in the center-of-mass system described by the expansion of the scattering cross section in a series of Legendre polynomials (formerly only the average value of the cosine of the scattering angle could be used). A code has been written which uses the coefficients of a given Legendre expansion and computes the probability of scattering at the angles which are zeros of the polynomial. All the additions were the result of requests by the Neutron Physics Division for aid in shielding research.

### Energy Depositions by High-Energy Nucleons

A program was written to study energy deposited in tissue by high-energy incident radiation as a function of depth and to separate various contributions to the energy deposited to determine which are the most important. Conversion factors were obtained to translate information about incident radiation into units which indicate the biological effects of higher-energy radiation.

The Nucleon Transport Code Group<sup>19</sup> was used to calculate the transport of normally incident high-energy protons or neutrons through 30- and 50-cm-thick slabs of infinite extent which are composed of a tissue-equivalent material.

Analysis codes were then written to obtain the contribution to the energy deposition as a function of depth in tissue by primary incident protons (if protons were the source particles), secondary cascade protons, evaporation protons, heavy evaporation particles, and residual nuclei that recoil after nonelastic interaction. The energy deposited by neutrons in elastic scattering events with nuclei was also calculated. Finally, the energy available for gamma-ray production through the decay of excited nuclei was obtained, along with an estimate of the capture gamma-ray production.

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<sup>19</sup>W. E. Kinney, R. R. Coveyou, and C. D. Zerby, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, pp 204-13.

Calculations have been performed for incident protons with energy from 100 to 400 Mev in 50-Mev steps. Two thousand protons were used in each case.

### Proton Dose Behind a Shield

A program was written to compute the dose due to protons behind an aluminum shield varying in thicknesses from 1 to 65 cm, in 2-cm steps. The flux at the various intervals was first computed, and then converted to dose (rad/hr) by interpolating within a table of conversion factors. Input to the code was from tapes prepared by O5R.

### Shielding for High-Energy Radiations

Output routines have been written for a program<sup>20</sup> which will develop high-energy electron-photon cascade showers in a homogeneous material with mixtures of up to 20 elements. The input data specifies the composition, and cross sections are set up automatically. The geometrical configuration may be a slab, a cylinder, or a cylindrical shell. The cascades can be initiated by positrons, electrons, or photons at any incident energy up to 50 Gev.

The results of the program include estimates of the track length for charged particles and for photons in each energy interval, radial interval, and depth interval. Fluxes are given in each energy interval at each radiation length of data to a depth of 10 radiation lengths. The calculation provides the energy deposited in each depth interval and radial interval and the energy spectra and angular distribution of the radiation penetrating the scattering medium if the medium has a finite thickness.

### Inelastic-Scattering Cross Sections

The  $0^+-2^+$  spin-orbit program<sup>21</sup> has been completed for the IBM 7090. It was designed to study the inelastic scattering of spin- $\frac{1}{2}$  particles to excited nuclear levels which are strongly coupled to the ground state. For incident protons the program computes the total absorption cross section, the total, inelastic  $2^+$  cross section, the elastic and inelastic differential cross sections, and the corresponding polarizations. For incident neutrons the total nuclear and total elastic cross sections are also given.

### Range-Energy Relationships for Protons

As part of the Apollo shielding program, it was required to know the range-energy relationship for protons penetrating NaI and other materials for which range-energy information was not readily available in the literature. To obtain this information the Bethe-Bloch equation, expressing differential energy loss as a function of energy, was coded for the computer. By solving this equation and integrating over appropriate limits, the amount of energy lost by protons penetrating thin materials and the total range of the protons could be determined as a function of material, thickness, and energy.

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<sup>20</sup>*Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, pp 248-60.

<sup>21</sup>B. Buck, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, p 83.

The main purpose of this program was to determine the response functions of NaI crystals used as detectors in the Apollo shielding experiments. However, the program was written in general terms so that it could be applied for nearly any material and any thickness.

### Orange Aid

This program was written for the IBM 7090 at Atomics International and tested at ORNL. The program is a Monte Carlo code with no provision for importance sampling. It is suitable, for example, for obtaining leakage spectra from a fairly small system.

In test problems the program appeared to yield results of proper magnitude. However, when the same problem was run several times with different starting random numbers, portions of the output would be found to be identical in two or more cases (beyond any reasonable statistical expectation).

Some time was spent in detecting the cause for this. The cause was finally determined to be the selection of the initial random number always from a limited sequence (500), the sequence being generated by the random-number generator with the first number of the sequence as input.

### The SNAP Program

A single scatter model for neutrons has been used to investigate the following SNAP problems:

1. The feasibility of measuring the effect on dose rate from neutrons scattered from integral components of SNAP configurations 10, 2, and 8;
2. The effect of air-scattered neutrons on SNAP experiments at the TSF;
3. The increase in dose rates at different payload locations from neutrons scattered off two different SNAP-50 radiators. Both radiators are in the preliminary design stage.

An IBM code has been written for each of the above problems, and the results have been published in another ORNL report.<sup>22</sup>

### Gamma-Ray Cross-Section Data

A system for generating detailed tables of gamma-ray cross-section data for any mixture of elements, as well as providing a means of rapid access to these data, has been devised for use on the IBM 7090 computer. The system, which was primarily designed for use in various Monte Carlo codes but can be easily used with other codes, consists of a master magnetic tape containing a limited amount of cross-section data, a code to update and edit the master tape, and a package of subroutines to generate detailed tables by using data on the master tape.

The use of the system is described elsewhere.<sup>23,24</sup>

<sup>22</sup>Space Power Program Semiannual Progr. Rept. Dec. 31, 1962, ORNL-3420 (to be published).

<sup>23</sup>S. K. Penny, M. B. Emmett, and D. K. Trubey, *A System for Generating Gamma-Ray Cross-Section Data for Use with the IBM-7090 Computer*, ORNL TM-234 (May 16, 1962).

<sup>24</sup>S. K. Penny, M. B. Emmett, and D. K. Trubey, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, p 89.

### The OGRE Code System

OGRE is a Monte Carlo code system for the IBM 7090 computer which is used for calculations of gamma-ray transport. The system is a skeleton program consisting of a number of subroutines that provide the basic framework of structure repeated in every Monte Carlo code dealing with gamma-ray transport. The advantage of such a program is that most types of gamma-ray codes can be "manufactured" by writing a few special subroutines, such as routines describing the source and the geometry.

Adaptations of the system to the calculation of gamma-ray dose rates and heating are described below.

A Monte Carlo program, OGRE-P1<sup>25,26</sup> was written within the framework of the OGRE system to solve the problem of the transmission of monoenergetic gamma rays through laminated slabs of various materials.

A Monte Carlo program, OGRE-P2,<sup>27,28</sup> was written within the framework of the OGRE system to solve the problem of gamma-ray leakage from a slab of laminated regions of various materials containing distributed sources.

A Monte Carlo code was written in the OGRE system to compute energy deposition by gamma rays in an infinite-slab geometry.<sup>29</sup> The slab may consist of 50 laminations, which in turn may consist of as many as 13 distinct homogeneous mixtures of elements.

### Scintillator Response

Minor program changes were made for a code written to measure the effect of delta rays on scintillator response.<sup>30,31</sup> Cases were run with the completed program, using new sets of data.

### Miscellaneous

About 20 special-purpose codes were written to perform shielding calculations for a complex engineered system. These codes involved complex manipulation of data, Monte Carlo calculations, and numerical integration.

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<sup>25</sup>D. K. Trubey, S. K. Penny, and M. B. Emmett, *OGRE-P1, A Monte Carlo Program for Computing Gamma-Ray Transmission Through Laminated Slabs*, ORNL TM-167 (Revised) (May 23, 1962).

<sup>26</sup>D. K. Trubey, S. K. Penny, and M. B. Emmett, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, p 90.

<sup>27</sup>D. K. Trubey, S. K. Penny, and M. B. Emmett, *OGRE-P2, A Monte Carlo Program for Computing Gamma-Ray Leakage from Laminated Slabs with a Distributed Source*, ORNL TM-237 (Aug. 10, 1962).

<sup>28</sup>D. K. Trubey, S. K. Penny, and M. B. Emmett, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, pp 91-94.

<sup>29</sup>S. K. Penny, D. K. Trubey, and M. B. Emmett, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1962*, ORNL-3360, p 94.

<sup>30</sup>*Math. Panel Ann. Progr. Rept. Dec. 31, 1961*, ORNL-3264, pp 42-43.

<sup>31</sup>For a more detailed discussion, see A. Meyer and R. B. Murray, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1961*, ORNL-3193, p 74.

## PHYSICS

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**Internal Bremsstrahlung Accompanying the  $\beta^-$  Decay of Helium-6<sup>32</sup>**

Approximately 300 internal bremsstrahlung (I.B.) and gamma-calibration spectra (of 180 channels each) were corrected, as necessary, for background counts and shifts in the energy calibration of the analyzer.

The I.B. spectra were divided into 5 groups corresponding to variations in the experimental conditions. Sums were found for subsets of these groups, which were related to finer variations in experimental differences (e.g., different beta-absorbing materials, or atomic number  $Z$ ).

These sums were corrected for a small amount of Ne<sup>23</sup> contamination in the He<sup>6</sup> gas by comparing the content of the 0.436-Mev gamma-ray peak in the I.B. spectrum with the corresponding peak's proportional part of a total Ne<sup>23</sup> calibration spectrum.

Finally, these sums were subjected, channel by channel, to least-squares linear fits, with  $Z$  as the independent variable, and the resulting curves extrapolated to zero  $Z$ .

An attempt to fit the pulse-height spectra resulting from these extrapolations by least squares before their conversion was unsuccessful.

**Fission-Fragment Experiments**

The experiment involves the use of surface-barrier detectors to measure energies of correlated pairs of fission fragments. Basically, data are accumulated event by event on paper tape. Sorting and summing routines produce an array of  $128 \times 128$  numbers which, when energy calibrations are applied, give the complete energy correlation spectrum for the fission fragments. Transformations are then made from this  $E_1$ ,  $E_2$  array to give distributions in fragment mass (from conservation of momentum) and total kinetic energy ( $E_K = E_1 + E_2$ ), and to give correlations of interest in the physics of fission, such as  $M_1, E_1$ ;  $M_2, E_2$ ;  $M_1/M_2, E_K$ . For each  $M_1$ , there results a frequency distribution of  $E_1$ , and similarly for the other pairs of variables, so that to extract the parameters of interest, plots are required of many of these distributions.

The data-processing techniques outlined above for the multiparameter experiments are new, and it has been of value to pursue some of the problems jointly with T. D. Thomas of Princeton University and Brookhaven National Laboratory. Data have been exchanged with Thomas and with W. M. Gibson of Bell Telephone Laboratories in an effort to arrive at the best possible procedures.

A correlated fission-fragment time-of-flight experiment is in final stages of assembly, and codes similar to those indicated above are being developed for these data. Thus far codes which give the mass distribution and the  $M_1, t_1$  correlations have been completed. For direct comparison of the two types of

<sup>32</sup>Math. Panel Ann. Progr. Rept. Dec. 31, 1961, ORNL-3264, p 41.

experiments, a code has been written to obtain time-of-flight spectra from the  $E_1$ ,  $E_2$  arrays. Codes have also been written to enable determination of the effect of prompt neutron emission by the fragments on these data.

### Transition Probabilities

In order to compute the transition probabilities from Ne states to  $\text{Na}^+$  states, a computer program was written. Part of the wave functions  $\psi_i(r)$  were supplied by tables of unequal intervals and some by means of formulas. The tables were interpolated in order to arrive at data over equal intervals. The  $\psi_i$  were normalized; that is,

$$\int_0^{\infty} \psi_i \psi_i dr = 1$$

The transition probabilities  $P_n$  were computed according to the formula

$$P_n = \left| \int_0^{\infty} \psi_f \psi_i dr \right|^2$$

Simpson's rule was used in both integral approximations.

### Relativistic Hartree Wave Functions for Many-Electron Atoms

Initial studies were begun during the period for a flexible and versatile program to calculate wave functions for many-electron atoms, using the Dirac relativistic wave equation and a Hartree self-consistent potential approximation.

### Mössbauer Spectra

The curve-plotting section of the code giving the velocity spectrum for the Mössbauer effect<sup>33</sup> was changed to use the Calcomp curve plotter.

A program has been written which takes data from measurements of Mössbauer spectra with applied magnetic fields and yields information related to nuclear magnetic moments. The process consists of smoothing background data with a nine-point smoothing formula, taking the quotient channel-by-channel of spectrum vs background, and then normalizing. The resulting set of points is then sometimes fitted to a Lorentz-type curve, using a nonlinear least-squares code.<sup>34</sup> The data are plotted so that the center section of the curve may be seen.

The program also handles measurements taken from analyzers which have paper-tape output.

<sup>33</sup>*Math. Panel Ann. Progr. Rept. Dec. 31, 1961, ORNL-3264, p 40.*

<sup>34</sup>*M. H. Lietzke, A Generalized Least Squares Program for the IBM 7090 Computer, ORNL-3259 (Mar. 21, 1962).*

### Mössbauer Effect in Small-Angle Reflection of Gamma Rays<sup>35</sup>

A program was written for the IBM 7090 for the calculation of the reflectivity of a mirror consisting of a nuclear resonant gamma-ray absorber (e.g., Fe<sup>57</sup>) for gamma rays incident at small angles and having energies in the neighborhood of the resonances of the mirror material. The program is designed to calculate reflectivity as a function of source speed for many values of source speed at a particular angle of incidence. Corrections for the finite angular spread of the experimental geometry and for the finite width of the source-energy distribution are included. Experience to date with the program has indicated that it is quite efficient; a set of corrected reflectivities can be calculated for 200 velocity values in about 1 min of computer time, including preparation of a magnetic tape for input to the Calcomp digital plotter.

### Calculation of Electron Density in Alloys

The small shift in nuclear transition energies resulting from changes in the density of electrons at the nucleus can be measured by the isomeric chemical shift observed in Mössbauer-effect experiments. The penetration factor, defined as the ratio of the electron density at the nucleus in an alloy to the electron density at the nucleus in the pure metal, has been obtained from a quantum-mechanical calculation of the scattering of a Fermi gas of electrons from the impurity atom. It has been assumed that the impurity atom can be regarded as a square well or barrier:

### E2 Coulomb-Excitation Calculations

A program was written for the IBM 7090 to investigate the E2 Coulomb excitation resulting from alpha-particle bombardment of very thick targets. This program is quite similar to one written for the Oracle.<sup>36</sup>

### Calculation of Clebsch-Gordan and Racah Coefficients

Two FORTRAN function subroutines for calculating Clebsch-Gordan and Racah coefficients were revised and corrected. These coefficients are extensively used in the theory of nuclear reactions.

The original routines were written by T. J. Kostigen, then with General Electric, and covered a range of 0! to 24!. The amended version, by means of  $\log(n!)$ , extended the range to 40!, and an error in computing the lower limit in the summation was detected and eliminated.

### Neutron-Diffraction Data Processing

Intensity data from neutron-diffraction experiments, initially punched in seven-channel paper tape, are transferred to magnetic tape using a program for the CDC 160-A computer. The data are supplied in ten-digit groups giving a channel number and the number of counts in the channel. A run consists of two tapes

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<sup>35</sup>S. Bernstein and E. C. Campbell, "Total Reflection of Gamma Rays over the Region of Nuclear Anomalous Dispersion in Fe<sup>57</sup>," paper presented at the Second International Congress on the Mössbauer Effect, Saclay, France, Sept. 13-15, 1961.

<sup>36</sup>*Math. Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, p 39.

unless there is an additional background tape. A program has been written for the IBM 7090 to calculate intensity differences, a corrected background (if a background tape is supplied), and an angle for each channel, beginning at the lowest channel common to all input tapes. These results are printed out and, in addition, may be plotted on the Calcomp digital plotter.

#### **Calculation of Coefficients of Fractional Parentage**

A program was written for the IBM 7090 to calculate coefficients of fractional parentage (cfp's) and related quantities useful in shell-model calculations of nuclear properties. The cfp's are the expansion coefficients in the expansion of the wave function for a system of  $n$  particles in terms of outer products of two wave functions, one for  $n_1$  particles and one for  $n_2$  particles with  $n_1 + n_2 = n$ . In the usual notation the  $n_1$  is dropped and the cfp's are referred to as  $n_2$ -cfp's for  $n$  particles, or  $n_2$ -particle cfp's. If all 1-cfp's are known, all other orders of cfp's may be evaluated from them, and in fact all quantities of physical interest in shell-model calculations for a given shell may be calculated if 1-cfp's are known.

Results of the calculations to date of 1-cfp's are available and publication of a tabulation of results is planned.

#### **Numerical Analysis of Neutron Resonances**

Additional computations and modifications were made in the computer programs described in ORNL-3205.<sup>37</sup> An addendum to this report has been written.

#### **Charged-Particle Cross-Section Compilation**

A program has been written to process differential cross-section data, excitation functions, and polarization data. It provides for coordinate transformations from the laboratory to the center-of-mass system and computes the ratio of the elastic cross section to the Coulomb (Rutherford) cross section if desired. The program provides for a reduction of analog values obtained from linear and semilog plots to absolute data. Energies of the reaction products in the laboratory system as well as the ratio of the solid angles in the laboratory to the solid angles in the center-of-mass system may be computed for two reaction products where appropriate.

A plotting subroutine is being written so that the data can be plotted for publishing. Also a more flexible printout is being incorporated to allow the computer printout to be used directly in the published compilation.

#### **Gamma-Ray Spectrum Fitting**

In the analysis of complex gamma-ray spectra the principal problem is the determination of a set of photon intensities from an observed set of counts in the channels of a multichannel analyzer, given the

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<sup>37</sup>Susie E. Atta and J. A. Harvey, *Numerical Analysis of Neutron Resonances*, ORNL-3205 (Dec. 26, 1961).

response of the experimental system to a selected set of monoenergetic gamma rays. Mathematically the problem may be stated as

$$Ra = c, \quad (1)$$

where  $a$  is a vector with  $N$  components giving the intensity of each gamma ray,  $c$  is a vector with  $M$  components giving the observed counts in each channel (or group of channels) of the multichannel analyzer, and  $R$  is an  $M \times N$  matrix giving the response of the system to a set of  $N$  monoenergetic gamma rays in each of the  $M$  analyzer channels. The system of equations is usually over-determined ( $M > N$ ) and the problem then is to find a "best" solution (in some sense). A program has been written for the IBM 7090 to find a linear least-squares solution to (1), given a tabulated response matrix  $R$ . Up to 14 gamma rays and 250 channels may be used. In addition the program can be used to find a set of intensities  $a_l$  and gain shifts  $s_l$  such that the elements of the response matrix for the  $l$ th gamma ray and  $j$ th channel is of the form

$$a_l \left[ F_{lj} + s_l \left( \frac{\partial F_l}{\partial \zeta} \right)_j \right], \quad (2)$$

where the derivatives  $\partial F_l / \partial \zeta$  may be tabulated or calculated by central difference of the  $F_{lj}$ . The direct-search procedure of Hooke and Jeeves<sup>38</sup> is used to solve for the  $s_l$ , using linear least squares to determine a set of  $a_l$  initially and after each pattern move. This procedure permits evaluation of a set of  $s_l$  bounded by input constraints, and is in addition quite efficient and easy to program.

An additional program was written for the IBM 7090 to calculate coefficients for an analytical fit of the response of the experimental system to monoenergetic gamma rays. A nonlinear least-squares procedure was used to obtain the coefficients in the form

$$y = \left[ C_0 + C_1 x^2 + C_2 x^4 + C_3 x^6 \right] \left[ 1 - e^{-b_6(x-b_7)} \right]^2 + a_1 e^{-b_1(x-x_{G1})^2} + a_2 e^{-b_2(x-x_{G2})^2}, \quad x \leq b_7; \\ y = a_1 e^{-b_1(x-x_{G1})^2} + a_2 e^{-b_2(x-x_{G2})^2}, \quad x \geq b_7.$$

### Energies of Low-Lying Levels in Br<sup>79</sup>

The energies of low-lying levels in Br<sup>79</sup> can be studied assuming that the last odd particle in one of three single-particle orbits is coupled to one of several collective states of the even-even core. The mathematical problem involved is that of diagonalizing a real symmetric matrix  $A$ . A program was written for the IBM 7090 to carry out such calculations.

### Circuits for Use with Superconducting Magnets

The solutions of systems of coupled ordinary differential equations describing proposed electrical networks were numerically approximated by the use of a Runge-Kutta fourth-order method. Some of the solutions gave good insight into the proper circuits to be used with superconducting magnets.

<sup>38</sup>Robert Hooke and T. A. Jeeves, "'Direct Search' Solution of Numerical and Statistical Problems," *J. Assoc. Comput. Mach.* 8, 212 (April 1961).

In a particular special case the time behavior of the current in a superconducting magnet is described by an equation of the form<sup>39</sup>

$$i(t) = 0.4847 \exp[-(a/2)(t - w/a)^2] \left\{ \int_0^t \exp[(a/2)(t' - w/a)^2] dt' + 41.262 \exp(w^2/2a) \right\}.$$

A program was written to find the value of  $t$  for which  $i$  is a maximum, given values of  $a$  and  $w$ .

### Computation of Eigenvectors

Several procedures were programmed for obtaining the eigenvectors from a symmetric matrix with known eigenvalues. Since the matrix and the corresponding eigenvalues were computed, both contained rounding errors. Difficulties experienced with these procedures were due to the computational errors and the nearly equal eigenvalues. The procedure which was found to give satisfactory results is an adaptation of the staircase method described in Chap. 7 of a forthcoming book.<sup>40</sup>

## REACTORS

Susie E. Atta	Nancy M. Dismuke
D. K. Cavin	D. A. Gardiner
Arline H. Culkowski	Jewel G. LaTorre

### Sodium Components Development

Statisticians in the Mathematics Division continued to cooperate with the Sodium Components Development Program Working Group of the USAEC. As members of the Ad Hoc Review Group for the General Electric Company's Mass Transfer Program, they tendered advice on the planning of experiments and assistance in the interpretation of statistical analyses.

### Analysis of Experimental Data from the Reactor in SPERT-I

Several attempts were made to obtain an approximate analysis of the experimental data observed during a series of self-limiting power-excursion tests of the SPERT-I oxide core<sup>41</sup> reactor.

The purpose of the analysis was to find the properties of the reactivity above prompt critical in dollars. This reactivity is composed of the reactivity originally inserted during the step-transient and the compensated reactivity. The originally inserted reactivity is determined from known parameters. The compensated reactivity is affected by the contribution of the Doppler coefficient, the contribution of the change in the number of water molecules, and the contribution of the fuel-rod bowing.

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<sup>39</sup>R. W. Boom and L. D. Roberts, "Study of the Transition of Small Niobium-Zirconium Superconducting Solenoids to the Normal State," paper to be submitted to the *Journal of Applied Physics*.

<sup>40</sup>A. S. Householder, *The Theory of Matrices in Numerical Analysis* (will be published in the near future).

<sup>41</sup>W. K. Ergen and A. H. Spano, "Effect of Fuel-Rod Bowing During Self-Limiting Power Excursions in the SPERT-I Oxide Core," presented at the American Nuclear Society Annual Meeting, Boston, Massachusetts, June 18-21, 1962.

Several computer programs were written to approximate the effects of these contributions. Some of the approximations gave quite accurate results; others were unsuccessful.

#### Reactor Power Spectrum Analysis

The Reactor Power Spectrum Analysis Program<sup>42</sup> was revised and rewritten for the IBM 7090. Added to the code were autocorrelation and cross-correlation options, as well as plotter options to graphically represent the output. The plotter options generate a tape which is plotted on the Calcomp 560R plotter, which gives the originator the overall results of the analysis along with the detailed output. The current program can handle two sets of points simultaneously, with a maximum of 6000 points per set. Changes are planned to generalize the program even further, and a report describing the revised program will be published.

#### ORR Fuel Inventory

The first section of this program<sup>43</sup> was written for the IBM 7090 for production after the shutdown of the Oracle. Additional bookkeeping procedures are being incorporated into a program for the CDC 1604-A to further simplify the paper work of Operations personnel.

A paper describing the program and its applications was presented at the Conference on Light-Water-Moderated Research Reactors by A. L. Colomb, the originator of the problem.

#### Sisyphus

Further checking and programming changes were done for Sisyphus,<sup>44</sup> a nuclear burnup code.

### REACTOR CHEMISTRY

G. J. Atta  
H. P. Carter

Arline H. Culkowski  
D. A. Gardiner

M. T. Harkrider  
R. P. Leinius

Mary J. Mader  
D. C. Ramsey

#### Analysis of BeO Grains

Consultation was provided to the investigator concerned with the analysis of BeO grains. Nonlinear models were fitted by nonlinear least-squares techniques to x-ray diffraction data, tritium diffusion data, and lithium diffusion data.

#### Beryllium Oxide Irradiation Experiments

Since the last report the experimental design for the BeO irradiation experiments<sup>45</sup> was completed and the experiment was begun. The experimental design was a 2<sup>5</sup> factorial experiment confounded in six replications. The two-level factors are pellet size, BeO density, grain size, temperature, and time of irradiation. A sixth variable, neutron flux, was introduced by confounding on the higher-order interactions. A complete description of the experimental design together with an explanation of the analysis has been published.<sup>46</sup>

<sup>42</sup>Math. Panel Ann. Progr. Rept. Dec. 31, 1961, ORNL-3264, p 41.

<sup>43</sup>Ibid., p 37.

<sup>44</sup>Ibid., pp 36-37.

<sup>45</sup>D. A. Gardiner *et al.*, Math. Panel Ann. Progr. Rept. Dec. 31, 1961, ORNL-3264, p 45.

<sup>46</sup>D. A. Gardiner, *The Experimental Design for BeO Irradiation Experiments* ORNL 41-8 and ORNL 41-9, ORNL-3310 (July 2, 1962).

### Analysis of French Iodine-Absorption Data

A nonlinear least-squares fit of some French iodine-absorption data for an empirical model was attempted. The iterative process failed to converge.

### Release of Fission Products

A program which converts the amount of activity represented by an isotope to an equivalent number of fissions occurring in a given time  $T$  has been completed. Corrections are made for decay of the isotope during time  $T'$ . From these data, the release from fuel specimens and from various volumes of the apparatus are calculated. The formula used for this analysis is

$$F = \frac{AT'}{C(1 - e^{-T'L})(e^{-TL})},$$

where  $A$  is the activity,  $T'$  the radiation time,  $C$  the fission yield,  $L$  the decay constant,  $T$  the decay time, and  $F$  the number of fissions.

Plots are made of activities vs sample sizes, where the sample is usually stainless steel. From these plots, diffusion constants and particle sizes are obtained. Fractionation plots are also made to establish relationships among isotopes. A linear regression analysis is optional on these sets of points.

The data from all experiments for a single year are stored on tape so that computations using data from different experiments are possible.

### Analysis of ATR Corrosion Data

The corrosion of aluminum leads to the formation of an adherent, insulating layer of corrosion products on the corroding surface. If heat is transferred across the corroding surface at a constant rate, the temperature of the aluminum increases as the layer of corrosion product increases in thickness. In tests sponsored by the Advanced Test Reactor Project, in which aluminum subjected to high heat fluxes (between 0.5 and  $2.0 \times 10^6$  Btu hr<sup>-1</sup> ft<sup>-2</sup>) was corroded by water, it was observed that the rate of temperature increase decreased with continued exposure. The time-temperature curves could be expressed by the relationship

$$T = T_0 + m\theta^p,$$

where  $T$  is the temperature of the aluminum at time  $\theta$ ,  $T_0$  is the aluminum temperature at the start of the test, and  $p$  and  $m$  are constants. From each of approximately 2000 sets of time-temperature data, the least-squares value of the exponent was determined. The average value of the exponent was 0.73, with a standard deviation of  $\pm 0.06$ . This term was independent of temperature and heat flux.

The value of  $m$  is temperature dependent. From preliminary analysis of the data it appears that  $\log m$  is a linear function of the reciprocal of the absolute temperature. Using a fixed value of  $p$  (as yet undecided) the  $m$  values will be calculated for each set of data and  $m$  will be expressed as a function of temperature. Also, the  $T - T_0$  (or  $\Delta T$ ) term can be related to oxide thickness, so that ultimately the relationship

between oxide thickness and temperature will be expressible by an empirical relationship of the form

$$X = A\theta^p \exp\left(\frac{-B}{T}\right),$$

where  $X$  is oxide thickness,  $\theta$  is time,  $T$  is temperature, and  $A$ ,  $B$ , and  $p$  are constants.

### Fission-Gas Release

In fission-gas-release experiments a number of routine calculations are made whenever a sample reading is taken. In order to speed up calculations, a computer program has been written to do the calculations for in-pile experiments B-9 and C-1. The data for three krypton and two xenon isotopes are taken from a 256-channel gamma-ray spectrum. From these data the number of atoms per second in the isotope release, and the fractional isotope release, are computed for each of the above-mentioned isotopes.

### SPECIAL SUBROUTINES

D. K. Cavin	Margaret B. Emmett
Arline H. Culkowski	Marjorie P. Lietzke
Robin E. Smith	

#### Interpolation

An interpolation routine TERPOL was checked out. It was also compiled and run on the CDC 1604-A. The routine does linear, semilog, and log-log interpolation.

#### Gaussian Integration

A Gaussian-integration package was checked out and converted to CODAP for use on the CDC 1604-A. This code allows for the possibility of performing a fourfold integral and for an optional number of points in the Gaussian quadrature. The CODAP version has not been completely checked out.

#### Stepwise Multiple Regression with Variable Transformations

This SHARE-distributed program by E. F. Efroymson of Esso Research and Engineering Company was reviewed and broken down into its basic steps to determine the methods used to include and exclude variables. A detailed description, along with some conclusions on the usefulness of the program, has been written by D. A. Gardiner, in a report entitled "A Statistician's Remarks on the 7090 Program, 'Stepwise Multiple Regression with Variable Transformations (ER MPR3),' by E. F. Efroymson."

#### Subroutine Package for Digital-Recorder Input-Tape Preparation

A set of subroutines supplied by California Computer Products, Inc., was revised for use on the IBM 7090 to prepare input tapes for the Calcomp Digital Incremental Recorder, described in the section, "Computer Operations," in this report. Extensive reprogramming of these subroutines is now in progress to make

them more efficient, more flexible, and easier to use. A package for the CDC 1604-A computer is now in final checkout, and a package for the IBM 7090 will be available soon after completion of the 1604-A version.

### Computer Program for Data Scaling and Plotting

A computer program has been written for plotting data with the Calcomp 570 digital plotter. The program is a FORTRAN subroutine, and one of its principal features is the ability to automatically scale floating-point data if desired. Scaling and plotting may be done for blank paper, permitting maximum-sensitivity scaling with a complete grid drawn by the plotter. If printed graph paper is used, major intervals must be spaced 1 in. or  $\frac{1}{2}$  in. apart. Titles and labels for graphs may be specified. A complete description of this routine with instructions for its use has been published.<sup>47</sup>

### Plotter Program

An IBM 7090 subroutine package<sup>48</sup> was written to facilitate the plotting of curves and points on logarithmic and semilogarithmic graphs using the Calcomp plotter. The subroutines accomplish the necessary computations and prepare a magnetic tape for use by the plotter.

### Lagrangian Interpolation

A FORTRAN subroutine package<sup>49</sup> was written for the purpose of generating a table of data by Lagrangian interpolation in a smaller table of data. There are three options for the type of interpolation: linear, semilogarithmic, and logarithmic. The number of points to be used for the Lagrangian scheme is optional.

## UT-AEC AGRICULTURAL RESEARCH LABORATORY

Nancy M. Dismuke	D. A. Gardiner
Manuel Feliciano	Marjorie O. Labhart

### Responses of Holstein Calves to Dietary Calcium, Phosphorus, and Vitamin D<sub>3</sub> as Measured by Response Surface Techniques

A three-dimensional central composite design as described by Box and Wilson<sup>50</sup> and Box<sup>51</sup> was conducted. Thirty male holstein calves were assigned to 15 diets in pairs. The diets varied in daily intake

<sup>47</sup>M. P. Lietzke and R. E. Smith, *Casper: A Generalized Program for Plotting and Scaling Data*, ORNL-3394 (Jan. 16, 1963).

<sup>48</sup>D. K. Trubey and Margaret B. Emmett, *An IBM-7090 Subroutine Package for Making Logarithmic and Semi-logarithmic Graphs Using the Calcomp Plotter*, ORNL TM-430 (Dec. 12, 1962).

<sup>49</sup>S. K. Penny and Margaret B. Emmett, *An IBM-7090 Subroutine Package for Lagrangian Interpolation* (to be published).

<sup>50</sup>G. E. P. Box and K. B. Wilson, "On the Experimental Attainment of Optimum Conditions," *J. Roy. Stat. Soc. B* 13, 1 (1951).

<sup>51</sup>G. E. P. Box, "The Exploration and Exploitation of Response Surfaces: Some General Considerations and Examples," *Biometrics* 10, 16 (1954).

of calcium (1.25 to 20 g), phosphorus (1 to 16 g), and vitamin D<sub>3</sub> (3 to 30,000 I.U.). Regression equations containing linear, quadratic, and interaction terms for 39 responses were calculated. These responses measured growth or various responses related to growth. Nineteen of the 39 responses measured were significantly affected by the dietary levels. All dietary combinations within the experimental range studied were calculated for different levels of response for these 19 responses. These combinations are shown in a graphic three-dimensional plot.

The equation used was

$$Y = b_0 + b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{11} X_1^2 + b_{22} X_2^2 + b_{33} X_3^2 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3,$$

where

$Y$  = measured responses,

$X_1$  = code value for calcium (calcium level in grams per day per calf),

$X_2$  = code value for phosphorus (phosphorus level in grams per day per calf),

$X_3$  = code value for vitamin D<sub>3</sub> (vitamin D<sub>3</sub> level in I.U. per day per calf),

$b$ 's = regression coefficients.

Interactions or responses of the seeds of various species to preirradiation, relative humidity, and radiation dose were investigated. In the first group of five species a quadratic equation similar to the one above was used. Here

$X_1$  = humidity,

$X_2$  = radiation dose,

$Y$  = measure of dry weight of seedlings.

One of the five deviated significantly from regression. However, with this design one could interpolate for all radiation dose and all humidities.

Data from five different species plus the one which deviated significantly in the previous case were studied. This time, a cubic component and all interactions were added. Thus

$$Y = b_0 + b_1 X_1 + b_2 X_2 + b_{11} X_1^2 + b_{22} X_2^2 + b_{111} X_1^3 + b_{222} X_2^3 + b_{12} X_1 X_2 + b_{112} X_1^2 X_2 + b_{122} X_1 X_2^2.$$

This equation described the deviant species from the previous study as well as three others. However, two of the species were not well described, and further refinements are in progress.

In both cases the Calcomp plotter was used to plot response contours.

## SYSTEMS PROGRAMMING

D. E. Arnurius	D. K. Cavin
Nancy A. Betz	E. C. Long
J. G. Sullivan	

### 1604-A Systems Programming

A peripheral processing system capable of driving any portion of the 160-A computer system at its maximum possible speed has been written and checked out. Among other options available are the normal ones: cards to tape; tape to cards; tape to printer; cards to printer. Work is continuing on combining any two of these normal uses so that they may go on simultaneously. At present it appears that in simultaneous operation, maximum speed can be realized on only one of the options while the other must proceed at a slower rate. [For example, if tape-to-printer operation drives the printer at its maximum rate of 1000 lines/min, the card-to-tape operation going on simultaneously could proceed at around 500 cards/min (maximum possible rate = 650 cards/min)].

The card-to-tape option will be able to handle many of the special characters used by ALGOL [ $\div$  ;  $\uparrow$  :  $\geq$   $\leq$   $<$   $\wedge$   $\vee$ ]. This means that codes can be written almost completely in the ALGOL reference language and that the output on the printer will also be almost completely in the ALGOL reference language.

The 1604-A CO-OP Monitor system received from CDC has been studied at some length. Where possible, changes have been made and checked which will reduce differences between the IBM system and our own. The accounting system has been rather completely revised in order to reflect our accounting needs. Several errors in the system have been corrected. It will be necessary to observe the system in operation before making extensive changes. At present, except for slight differences in the FORTRAN languages between IBM and CDC, it would appear that there will be no difficulty in running codes on either machine.

### Programs for Processing Data Recorded on Paper Tape

Two programs for the initial processing of data recorded on paper tape were written for the 160-A computer. Although the programs were designed for use in separate problems, the same technique, a table-lookup procedure, was used in both. Each entry in the table determined the parity correctness or legality of the character read. This procedure is very fast and also affords great flexibility in the processing of paper tapes which have uniform anomalies.

### Oracle Simulator

Codes written for the Oracle were reprogrammed for the IBM 7090 computer on request by the users. The use of the Oracle Simulator<sup>52</sup> for the CDC 1604-A computer was obviated and further work discontinued.

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<sup>52</sup>*Math. Panel Ann. Progr. Rept. Dec. 31, 1961, ORNL-3264, pp 12-14.*

## COMPUTER OPERATIONS

H. P. Carter	S. O. Smith
Edith M. Hogan	G. H. Stakes
E. C. Long	C. S. Williams

### The Oak Ridge Automatic Computer and Logical Engine (1953-1962)

The Oak Ridge Automatic Computer and Logical Engine (Oracle) was designed at Argonne National Laboratory and installed at ORNL in 1953. Initially the machine was equipped with a cathode-ray tube memory with a capacity of 1024 40-bit words and a cycle time of 18  $\mu$ sec. Input and output were on five-channel paper tape, providing the numerals zero through nine and alphabetic characters A through F. The computer performed fixed-point binary arithmetic with an add time of 70  $\mu$ sec.

In 1955, four magnetic-tape units were added to the computer to provide auxiliary storage. These units used 2-in.-wide Mylar plastic tape with a packing density of 90 Oracle words per inch and an effective transfer rate of 2500 words per second. The information on the tapes was recorded twice, resulting in very high reliability of operation.

In 1956, a cathode-ray tube curve plotter, which was designed and built by ORNL engineers, was added to the computer as an auxiliary output device. Automatic character plotting, not available on other computers until 1959, was included so that the curve plotter could be used for digital output, affording an efficient means for the output of large batches of data.

In 1957, the console was redesigned and rebuilt, and extensive additions were made to the input-output equipment. The input tape was enlarged to seven channels, permitting the use of an extended alphabetic and numeric character set, and a console typewriter and a narrow magnetic-tape output unit were added. Additional computer instructions for the control of the new input-output devices were added to the basic instruction set, and the capacity of the cathode-ray tube memory was doubled to 2048 40-bit words.

In 1961, an additional magnetic tape was added to the computer to enable reading and writing of tapes compatible with IBM equipment.

A number of subroutines and service programs were written for the Oracle, and reports of these were distributed to machine users at the Laboratory. In addition, three compilers were written for the computer. The first of these was principally an assembler designed to simplify storage allocation. The second compiler program, ORBIT (Oak Ridge Binary Internal Translator) was a translator to produce machine-language programs from programs written in a special source language. The third program was a translator to produce machine-language programs from programs written in a dialect of ALGOL 58.

Due to the rapidly expanding needs of the Laboratory for high-speed computing equipment, the Oracle was dismantled in the fall of 1962 and is to be replaced by a Control Data Corporation 1604-A computer, a modern transistorized digital computer with 32,768 48-bit words of ferrite-core memory having an effective cycle time of 4.8  $\mu$ sec.

During the existence of the Oracle, more than 32,700 hr of computing time was logged, with more than 1,000 separate problem charges.

### Oracle Time Use

The operation of the Oracle is specified by the total number of hours of computing time, defined as the number of hours in which the computer was used for production runs or in problem checking. Repairs, machine testing, and idle time available but not used are not included in the total. The following table summarizes the operation of the Oracle during its existence.

Year	Computing Time (hr)	Monthly Average (hr)
1954	1,685	140
1955	3,496	291
1956	4,825	402
1957	3,892	324
1958	5,420	452
1959	4,969	414
1960	4,203	350
1961	2,868	239
1962	<u>1,311</u>	146
	32,769	

Operation of the Oracle in 1962 is summarized in the table below.

Month	Computing Time (hr)	Check-Out (hr)	Production (hr)
January	128:40	26:22	102:18
February	147:08	33:26	113:42
March	151:53	28:54	122:59
April	195:52	18:41	177:11
May	142:33	17:05	125:28
June	123:01	1:18	121:43
July	207:11	:17	206:54
August	143:46	1:21	142:25
September	<u>70:52</u>	<u>1:30</u>	<u>69:22</u>
	1310:56	128:54	1182:02
Monthly av	146:11	14:28	130:22

### Digital Recorder

A Calcomp<sup>53</sup> Digital Incremental Recorder and a model 570 magnetic-tape transport were purchased and placed in operation. Input tapes for the recorder are prepared on a digital computer and later processed by the recorder, so that the digital computer does not drive the recorder directly. This procedure saves computer time and has the additional advantage that tapes prepared on different digital computers may be used as input to the recorder, provided that the information is arranged in the proper format. A set of subroutines for this purpose for the IBM 7090 has been written and is discussed elsewhere in this report.

Since the recorder is digital in operation the problems of drift, dynamic response, and gain and scale-factor settings which occur with analog recorders are avoided. The recorder pen can be moved in 0.01-in. increments in the positive or negative *y* direction, and the paper transport can be moved in 0.01-in. increments in the positive or negative *x* direction. The tape transport provides the additional feature of searching for any particular graph on an input tape, so that graphs may be plotted in any desired order, regardless of their order on the input tape.

### Operating Services

A problem-setup service has assumed the responsibility of preparing and running computer problems of routine nature for users at the Laboratory.

The operating section which was responsible for running the Oracle is now responsible for the operation of the Calcomp curve plotter and will be responsible for the operation of the CDC 1604-A computer.

The keypunch section, which has been expanded during the year, provides keypunching service to the Laboratory.

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<sup>53</sup>California Computer Products, Inc.

## TRAINING COURSES

### Statistics Lecture Series

Between January 11 and March 15, 1962, members of the Statistics Group offered a series of nine lectures on "A Basic Course in Mathematical Statistics." The series, presented in Building 4500 at ORNL, was open to all interested personnel in Oak Ridge. It was designed specifically for persons of mathematical propensity with an interest in statistics. Prepared lecture notes were distributed to the participants at the conclusion of each lecture. The participation of 150 to 250 employees in each of the nine lectures is indicative of the success of these lectures.

The lectures and their contents are listed below:

**Lecture I** (D. A. Gardiner). – Introduction: The Question Posed by a Series of Numbers, Review of the Notation of Sets. Probability: The Three Axioms, The Six Basic Theorems, Definition of the Random Variable.

**Lectures II, III, and IV** (D. G. Gosslee). – Probability Density Functions: Their Characteristics, The Binomial Probability Density Function, The Poisson Probability Density Function, The Normal Probability Density Function. Mathematical Expectation: Moments of Probability Density Function, Means of Distributions, Variances of Distributions. Point Estimation of Population Parameters by Sample Statistics: Properties of Estimators, Methods of Obtaining Estimators.

**Lectures V, VI, and VII** (M. A. Kastenbaum). – Derived Sampling Distributions: Distribution of the Sample Mean and Sample Variance, The Central Limit Theorem, The Chi-Square Distribution, "Student's" *t* Distribution. Interval Estimation: The Construction of Confidence Intervals, Confidence Probabilities. Hypothesis Testing: Type I and Type II Errors, The Concept of Power, Simple and Composite Hypotheses, The Likelihood-Ratio Criterion.

**Lectures VIII and IX** (D. A. Gardiner). – Linear Regression: The Method of Least Squares, Minimum Variance Unbiased Estimates, Maximum Likelihood Estimates. Nonlinear Regression: The Generalized Newton Method, A Method Described by Garwood; Conclusion.

### ALGOL Lecture Series

A two-week lecture series by Manuel Feliciano, held in June 1962, was intended to introduce beginners to programming techniques using ALGOL. Special attention was given to the restrictions to the language of the CDC 1604-A version of ALGOL as well as that of the IBM 7090. Approximately 50 persons attended the series.

### FORTRAN Lecture Series

A two-week lecture series by Nancy B. Alexander, intended to give small audiences a working knowledge of FORTRAN 62 for the CDC 1604-A, was offered monthly, starting in August. Material covered in each series included a discussion of building blocks, basic statements (of input and output in particular), and declarations. In addition the concepts of program, subroutine, and fractions were treated. Throughout the series attention was given to the actual steps required to prepare, check out, and run a program in the local computing facilities. These lecture series were attended by approximately 100 persons.

## LECTURES AND PAPERS

Bumgarner, L. L., "Some Remarks on the Implementation of ALGOL," USAEC Computer Information Group Meeting, Gatlinburg, Tennessee, May 11, 1962.

Carpenter, J. A., "The Use of Involutory Matrices for Generating Matrix Test Data," Mid-Southeastern Chapter of the Association for Computing Machinery, Nashville, Tennessee, November 1962.

Carter, H. P. (with A. C. Downing and Joan Rayburn), "Calculation of the Shim Contours for the 255° Isotope Separator," Mid-Southeastern Chapter of the Association for Computing Machinery, Chattanooga, Tennessee, February 1962.

Cavin, D. K. (with A. L. Colomb), "Fuel Cycles and Loading Programming for Water-Cooled Research Reactors," Conference on Light-Water-Moderated Research Reactors, Gatlinburg, Tennessee, June 11-14, 1962.

Downing, A. C., "A Novel Finite-Difference Formulation for Multiregion Diffusion Problems," British Computer Society Annual Conference, Cardiff, Wales, September 1962.

Downing, A. C., "A Finite Green's Identity and Methods for Handling Interface Problems," National Physical Laboratory, Teddington; National Institute for Research in Nuclear Science, Harwell, September 1962.

Downing, A. C., "A Critical Analysis of Computers Available in the USA," Johannes Gutenberg-Universität, Mainz, Germany, August 1962.

Feliciano, Manuel, Jr., "The Effects of ALGOL on Programming," Southeastern Regional Meeting of the Association for Computing Machinery, Ft. Walton Beach, Florida, September 20-21, 1962.

Gardiner, D. A., "The Statistical Response Surface and an Example of Its Application," University of Florida, Gainesville, March 1962.

Gardiner, D. A., "Experiences with Experimental Design at Oak Ridge National Laboratory," Florida State University, Tallahassee, March 1962; Pittsburgh Chapter of American Statistical Association, Pittsburgh, November 1962.

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