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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

FOR

PERIOD ENDING DECEMBER 31, 1954

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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

for

Period Ending December 31, 1954

A. S. Householder, Chief
W. C. Sangren, Editor

DATE ISSUED

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MATHEMATICS PANEL SEMIANNUAL PROGRESS REPORT

INTRODUCTION

THE ORACLE

From July through December, a total of 1750 hr of computer time was used by programmers in "debugging" and in running problems. With the acquisition of a second operator, the evening shift was initiated. A night-shift operator is presently being trained, and third-shift operations will probably begin after completion of the magnetic-tape memory.

Engineering time is regularly scheduled for 4 hr each morning and ½ hr late in the afternoon. An electronic technician is on duty during evening-shift operations.

Installation of the magnetic-tape memory units is complete, and the units are expected to go into operation in the near future. Work is continuing on the new input-output system.

LECTURES

ORINS Lectures. One lecture was given under the Traveling Lecture Program as follows:

W. C. Sangren, *Solving Problems with the Oracle,* Georgia Institute of Technology, Oct. 7, 1954.

Other Lectures. Other lectures given during the report period are as follows:

J. Z. Hearon, *Integral Equations in Physiological Kinetics,* advanced course in uses of radioactive isotopes in biochemistry sponsored by ORINS, Sept. 17, 1954.

A. S. Householder, *Generation of Error in Computations with Continued Fractions,* International Congress of Mathematicians, Amsterdam, Sept. 4, 1954; *On Solving Linear Algebraic Systems,* Cambridge University, Sept. 30, 1954; *Norms of Vectors and Matrices,* meeting of the American Mathematical Society, Tuscaloosa, Alabama, Nov. 27, 1954.

F. W. Stallard, *Differential Systems with Interface Conditions,* meeting of the American Mathematical Society, Tuscaloosa, Alabama, Nov. 27, 1954.

A. W. Kimball, *Short-Cut Formulas for the Exact Partition of Chi-Square in Contingency Tables,* annual meeting of the American Statistical Association, Montreal, Canada, Sept. 10–13, 1954; *The Design of Chemical Experiments,* ORNL Chemistry Division Seminar, Oct. 6, 1954.

MEETINGS

The Second Southern Regional Conference on Statistics was held at Roanoke, Virginia, on July 8–10, 1954. This conference was sponsored by the Southern Regional Education Board; A. W. Kimball was the chairman of the Committee on Statistical Consulting Services during the conference.

LIST OF PUBLICATIONS

W. L. Russell, L. B. Russell, and A. W. Kimball, "The Relative Effectiveness of Neutrons from a Nuclear Detonation and from a Cyclotron in Inducing Dominant Lethals in the Mouse," *Am. Naturalist* **88**, 269–286 (1954).

A. W. Kimball and A. S. Householder, "A Stochastic Model for the Selection of Macronuclear Units in *Paramecium* Growth," *Biometrics* **10**, 361–374 (1954).

A. W. Kimball, "Short-Cut Formulas for the Exact Partition of X^2 in Contingency Tables," *Biometrics* **10**, 452 (1954).

S. D. Conte and W. C. Sangren, "An Expansion Theorem for a Pair of Singular First-Order Equations," *Can. J. Math.* **6**, 554–560 (1954).

A. S. Householder, *On Norms of Vectors and Matrices*, ORNL-1756 (Aug. 26, 1954).

A. S. Householder, *On Solving Linear Algebraic Systems*, ORNL-1785 (Sept. 21, 1954).

A. S. Householder, "Generation of Error in Computations with Continued Fractions" (abstract), p 354, *Proc. Intern. Congr. Math.*, Amsterdam, 1954.

A. S. Householder, "Generation of Errors in Digital Computation," *Bull. Am. Math. Soc.* **60**, 234–247 (1954).

J. Z. Hearon, "The Approach to Stationarity in Open Reaction Systems," *Arch. Biochem. and Biophys.* **51**, 43 (1954).

J. Z. Hearon and R. Katzman, "Enzyme Kinetics: Inhibition Equations Derived from the Inelastic Collision Hypothesis," *Bull. Math. Biophys.* **16**, 259 (1954).

EMPLOYEE CHANGES

R. C. Weaver terminated during this period; new employees were M. E. Fulmer and C. L. Bradshaw. G. L. Broyles joined the Panel as an operator for the Oracle, and W. G. Howe joined as an ORINS Fellow. Joining the Panel as a research participant was R. C. F. Bartels from the University of Michigan. Research participants who have completed their work with the Panel are N. Macon, N. Heerema, and W. R. Mann. M. Hochdorf from TVA is with the Panel as a loanee.

TRAINING COURSE

A series of lectures on programming for the Oracle was given for a period of six weeks beginning Nov. 15. The following topics were discussed:

A Survey of Programming
Logical Approach to Programming and the Oracle Operations
Oracle Operations in Detail
The Scaling Problem
Introduction to Machine Logic
Description and Use of Some Subroutines

Time was available on the Oracle for the training of those attending the lectures. A new series of lectures will be given whenever there is sufficient interest. Additions to the *Manual for the Oracle*, suitable for use with such a lecture series, will be made.

MATHEMATICAL RESEARCH AND SUBROUTINES

PROGRESS OF THE ORACLE SUBROUTINE LIBRARY

References: Mathematics Panel Quarterly Progress Reports, ORNL-1498, -1435;
Mathematics Panel Semiannual Progress Reports, ORNL-1588, -1662, -1751

Background and Status. With working codes now available for the elementary mathematical functions and for many of the most-needed higher functions, a greater amount of effort has been devoted to problems of optimal coding and of approaching as closely to automatic coding as present conditions will allow. Wherever possible, all routines are being evaluated in terms of speed, accuracy, ease of operation, and length. It is generally impossible to produce a single subroutine for a given purpose which is optimal in all these respects; consequently, several programs may exist for the same purpose, each program being optimal in some respects, and the choice of which one should be used in a given problem is left to the discretion of the programmer. The ability of the programmer to choose wisely is predicated upon the existence of accurate information about these characteristics of the available subroutines.

This situation particularly holds with respect to arithmetic-type codes. There are now in use five basic floating-point subroutines, which may be used in a total of nine different (packed or unpacked) forms. Each of these codes is optimal in some respect, and, in general, each one requires its own system of subroutines (although some of the floating-point subroutines are independent and will work in any floating-point code).

Also in the arithmetic category are the double-precision and complex arithmetic subroutines, which operate on the same set of instructions as some of the floating-point subroutines.

In addition to the subroutines designed to calculate various functions, there are several which calculate functionals. These include, in particular, four quadrature subroutines, two differential equation subroutines, and a number of matrix and determinant subroutines. These subroutines reduce the technical numerical problem of performing the indicated operation upon a function essentially to the problem of computing the function itself, just as the ordinary subroutine reduces the problem of evaluting $f(x)$ to the problem of determining what x is. In this same category belong Monte Carlo techniques, which may lend themselves to block coding methods.

The creation of an adequate set of such arithmetic, function, and functional subroutines appears to be a desirable prerequisite for the creation of automatic or semi-

automatic coding procedures. The possibility of using such procedures on the Oracle is being investigated, although the actual implementation of such a program depends upon the existence of magnetic tapes.

As soon as testing is complete, reports upon the various categories of subroutines will be issued; such reports will be designed to help the programmer decide which subroutine or subroutine system is best in terms of a particular problem. It is presupposed that all applicable methods would be examined thoroughly in the case of each subroutine, and those which are not optimal in some respect should be discarded.

MATRIX OPERATIONS[1,2]

Participating Members of Panel: N. Heerema, J. W. Givens, A. C. Downing, R. A. Willoughby, A. S. Householder

The purposes of this study are to develop and evaluate routines for performing the standard operations with matrices and, where possible, to extend the theory of matrices as it relates to numerical manipulation. The present section will be concerned primarily with basic theory, and although particular routines will be discussed elsewhere, a few general remarks will be made here concerning them.

Routines for solving systems of equations or inverting matrices may be assessed by a variety of conflicting criteria, and hence no single routine will be optimal for all purposes. Whether or not the matrix is large enough to require the use of tapes; whether or not it is symmetric or, if symmetric, is positive definite; whether or not high accuracy is required, so that perhaps an initial approximation may require iterative improvement; these and other considerations will govern the preference for one routine over another in any given case. Consequently, several different equation-solving and matrix-inverting routines are being or have been set up. The simplest is a Seidel iteration accelerated by application of Aitken's δ^2 process. In principle, the δ^2 process should convert the iteration to convergence, even when the simple iteration diverges, provided that the process is not applied too soon. However, if divergence is too rapid, scaling difficulties may interfere. Also, in principle, if the simple iteration converges, it should yield optimal accuracy.

Of the direct methods, the simplest is probably straight elimination, with no account taken of possible symmetry of the matrix, and, at each step, a search down the column for the largest element for use as pivot. This method is being used very effectively, but it is slow for inversion, since it must be applied n times.

A direct method applied to an ill-conditioned matrix could fail altogether or might yield a result that requires improvement by iteration. The standard iteration, with

[1] J. W. Givens, *Numerical Computation of the Characteristic Values of a Real Symmetric Matrix*, ORNL-1574 (Feb. 19, 1954).

[2] A. S. Householder, *Norms of Vectors and Matrices*, lecture presented at meeting of the American Mathematical Society, Tuscaloosa, Alabama, Nov. 27, 1954.

second-order convergence, is the following: If C_0 is approximately equal to A^{-1}, then $C_1 = C_0(2I - AC_0)$ is (apart from rounding errors) a better approximation to A^{-1}.

The conjugate gradient method of Stiefel and Hestenes for positive definite matrices modifies the Seidel iteration in such a way that, apart from rounding, an exact solution is obtained in not more than n iterations. The iterations are, of course, somewhat more complicated. While the result at the nth step will not be exact, in general, because of rounding errors, subsequent improvement by iteration is possible. The method is being programmed, although it appears that scaling is rather difficult and that storage requirements are heavy.

A method which seems not to be described in the literature is based upon the simple theorem that if A is any square matrix, there exists an orthogonal matrix D such that PA is triangular. Further, P can be generated as the product of $n(n - 1)/2$ plane rotations. There seems to be evidence that the generated error is less from the rotational triangularization than from more standard methods, and it might therefore be well adapted to the inversion of large matrices. The method is being programmed for use with tapes.

Consideration is being given to another method for arbitrary matrices that represents a kind of generalization of the conjugate gradient method. The method has some theoretical interest even if it should prove to be unsuitable for the Oracle. The system $Ax = b$ can be interpreted as requiring the resolution of the vector b along the columns of A. Given any vector x_0, regarded as approximating the solution x, a vector v_1 can be selected arbitrarily, and the residual $r_0 = b - Ax_0$ can be projected orthogonally upon $u_1 = Av_1$. When this projection is adjoined to x_0, the resulting vector x_1 yields a residual $r_1 = b - Ax$, which cannot be greater than r_0 and will, in general, be less (in terms of length). The process can be repeated indefinitely to yield a sequence of vectors x_p that converges to the true solution (disregarding generated errors) when A is nonsingular, and, when A is singular, the sequence converges to a vector orthogonal to the columns of A.

The infinite iteration is readily converted into one which terminates in, at most, n steps as follows: Each residual r_p is orthogonal to $u_p = Av_p$. Hence it is possible to start with $x_0 = 0$ and an arbitrary v_1, then take v_2 so that u_2 is orthogonal to u_1, v_3 so that u_3 is orthogonal to u_1 and u_2, ... Then $r_n = 0$ if A is nonsingular, and if A is singular, at some stage, the least-squares solution has been obtained, and subsequent steps bring about no change.

Actually, because of rounding errors, the process will not terminate strictly. However, the approximate solution can be improved by projecting again upon some of the vectors u_1, u_2, . . . already formed, and these vectors will be optimal for the purpose in the sense that they are nearly, although not strictly, orthogonal.

While the method has been described as one for solving a system of equations, it turns out that by storing suitable by-products, the inverse can be formed as a matrix product when A is nonsingular. Furthermore, if A is singular or very poorly conditioned, the fact becomes evident in the course of the computation, and a least-squares solution is obtained instead.

The method can be dualized by orthogonalizing the rows of A instead of the columns, although the result achieved in the singular case seems less useful. Estimates of the ultimate accuracy achievable by either method on continued projection have been worked out.[3]

The convergence of any iterative method can be made to depend upon the vanishing of a certain sequence of matrices, and often these matrices are powers of a fixed matrix. Convergence criteria can be phrased in terms of latent roots, which are generally unknown, or in terms of some norm which, although readily computed, may constitute an unnecessarily strong condition and hence provide a weak theorem.

A norm of a vector is a continuous function of the elements, positively homogeneous of first degree, and satisfies the triangular inequality. A norm of a square matrix is similarly defined, with the additional requirement that the norm of a product shall not exceed the product of the norms. A matrix norm $||A||$ is consistent with a vector norm $||x||$ if for every matrix A and vector x, $||Ax|| \leqq ||A|| \cdot ||x||$; and it is subordinate if for any A there exists an $x \neq 0$ for which equality holds. A subordinate matrix norm has the important property that $||I|| = 1$. In any event, for any H, if a norm can be defined in such a way that $||H|| < 1$, then the sequence $H^p \to 0$, and a measure of the rate of convergence when the condition is satisfied is measured by the magnitude of $||H||$. Hence it is desirable to be able to find a norm that is as small as possible for any given H.

In the literature there seem to have been defined only three norms, one of which requires the computation of a latent root. Of the other two, one is the maximum row-sum of absolute values and is called the e norm, $||x||_e$ and $||A||_e$; the other, the maximum column-sum of absolute values, is called the e' norm, $||x||_{e'}$ and $||A||_{e'}$. However, given any norm, $||x||$ or $||A||$, and a nonsingular matrix G, it can be shown that $||x||_G = ||G^{-1}x||$ and $||A||_G = ||G^{-1}AG||$ are also norms. Particular interest attaches to the case when G is a diagonal matrix of positive elements and either the e norm or the e' norm can be chosen. It is possible to obtain immediate generalizations of certain classical convergence theorems.[4] To show that the generalizations are nontrivial, it is sufficient to note that for the matrix $\begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}$, the e norm and the e' norm both equal

[3] A. S. Householder, *On Solving Linear Algebraic Systems*, ORNL-1785 (Sept. 21, 1954).

[4] A. S. Householder, *On Norms of Vectors and Matrices*, ORNL-1756 (Aug. 26, 1954).

$|\lambda| + 1$, whereas it can be shown that a norm exists whose value is $|\lambda| + \epsilon$, for any $\epsilon > 0$.

CALCULATION OF CHARACTERISTIC VALUES AND CHARACTERISTIC VECTORS OF A SYMMETRIC MATRIX

Origin: J. W. Givens

Participating Members of Panel: J. W. Givens, V. C. Klema

Background and Status. Five Oracle programs for symmetric-matrix calculations now exist in the Panel and can be listed as follows:

1. reduction of a symmetric matrix to the Jacobi form,
2. modified reduction of a symmetric matrix to the Jacobi form (this program records the $\sin\theta$–$\cos\theta$ pairs used in the rotation that are necessary for the characteristic vector computation),
3. calculation of characteristic values from the Jacobi matrix,
4. computation of characteristic vectors of the Jacobi matrix,
5. unrotation of the Jacobi matrix vectors to the characteristic vectors of the original matrix.

The first code (1) limits n, the order of the matrix, to be not greater than 32.

TRIANGULARIZATION OF A MATRIX BY ROTATIONS

Origin: J. W. Givens

Participating Members of Panel: J. W. Givens, V. C. Klema

Background and Status. Given a matrix A of m rows and n columns, it is desired to write an Oracle code to produce a matrix of the same size but with the (i,j) element equal to zero when $i > j$. The method is to make a sequence of plane rotations resulting in a matrix of the following form:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ & a_{22} & a_{23} & \cdots & a_{2n} \\ & & a_{33} & \cdots & a_{3n} \\ & & & \cdots & \\ & & & \cdots & a_{mn} \end{pmatrix} .$$

This calculation is to be programmed by using magnetic tape, and it is suggested that $m \leq 63$.

GAUSS-SEIDEL METHOD OF SOLVING SIMULTANEOUS LINEAR EQUATIONS

Participating Members of Panel: A. C. Downing, E. C. Long

Background and Status. A method of solving simultaneous linear equations by the Gauss-Seidel method has been programmed. Since this method is useful mainly for positive definite systems, Aitken's δ^2 process has been incorporated to accelerate

convergence. Programming of this method is complete, but a recoding will be accomplished when the magnetic-tape memory is available.

CONTINUED FRACTIONS[5]

Participating Members of Panel: N. Macon, A. S. Householder

Continued fractions seem not to have been used extensively in digital computation, in spite of the fact that certain transcendental functions have quite simple continued-fraction expansions which converge in regions where the standard power series do not. In fact, in classical analysis, continued fractions are often used for summing divergent series. Moreover, there exists a technique for expanding an arbitrary analytic function into a continued fraction in a manner analogous to the Taylor expansion into a power series. One difficulty, which is also an advantage, with the use of continued fractions lies in the multiplicity of equivalent forms of what is essentially the same continued fraction. Several subroutines have been constructed in which continued-fraction expansions were used, and studies are being made of errors generated in the course of various computational procedures.

If the fraction is in the form

$$F = b_0 + a_1/b_1 + a_2/b_2 + \cdots ,$$

then

$$F_i = b_0 + a_1/b_1 + \cdots + a_i/b_i = \frac{A_i}{B_i}$$

is called the ith approximant. It can be assumed that $|F| < 1$, since, otherwise, the reciprocal would be computed. In continuant notation,

$$A_i = K\begin{pmatrix} a_1, \cdots, a_i \\ b_0, b_1, \cdots, b_i \end{pmatrix} = K\begin{pmatrix} a_i, \cdots, a_1 \\ b_i, b_{i-1}, \cdots, b_0 \end{pmatrix},$$

$$B_i = K\begin{pmatrix} a_2, \cdots, a_i \\ b_1, b_2, \cdots, b_i \end{pmatrix} = K\begin{pmatrix} a_i, \cdots, a_2 \\ b_i, b_{i-1}, \cdots, b_1 \end{pmatrix}.$$

The A_i and B_i satisfy well-known recursion relations and, according to the K form used, may be corresponding terms with different initial conditions, or consecutive terms of the same recursion from the same initial conditions. Scaling is made possible by the identity

$$K\begin{pmatrix} c_0c_1a_1, \cdots, c_{i-1}c_ia_i \\ c_0b_0, c_1b_1, \cdots, c_ib_i \end{pmatrix} = c_0c_1 \cdots c_i K\begin{pmatrix} a_1, \cdots, a_i \\ b_0, b_1, \cdots, b_i \end{pmatrix}.$$

[5] A. S. Householder, *Generation of Error in Computations with Continued Fractions*, lecture presented at International Congress of Mathematicians, Amsterdam, Sept. 4, 1954.

Bounds can be given for the buildup of generated error in the evaluation of any continuant. These are linear combinations of the errors generated in the individual steps, the coefficients being themselves continuants whose elements are the absolute values of the a_i and b_i. In evaluating a continuant of order n, the coefficient of the error generated at the ith step is a continuant of order $n - i$ and may therefore increase quite rapidly with n.

If

$$D_n = b_n ,$$

$$D_{i-1} = b_{i-1} + \frac{a_{i-1}}{D_i} ,$$

then

$$D_0 = F_n .$$

This method of evaluation requires the selection of n in advance, but this is often quite feasible. It turns out that, in a large class of cases, the scale factors c_i can be selected in a rather simple way as powers of 2, and then an upper bound for the generated error, *independent of* n, can be given. Moreover, this bound is often small. Thus with digital x, the bound is 6ϵ for tan x and is 4ϵ for $\tan^{-1} x$, tanh x, log $(1 + x)$, and exp x, where $\epsilon = 2^{-40}$. Since taking n large involves no penalty in the form of increased generated error, the residual error can be made negligible, as compared with the generated error.

An ORNL report summarizing this work is now in preparation.

NUMERICAL INTEGRATION

Participating Member of Panel: C. L. Gerberich

In order to speed the processing of small integration problems, a series of subroutines has been written and used with great success. A problem that once might have required weeks can now be turned out in a matter of days. After considerable testing, it was found that the best all-round program was based on the Gaussian method of numerical integration. Since for a good programmer the scaling of an integral is a relatively simple job, the series of subroutines is in "fixed-point" form. At some later date it is hoped to recode this series in floating-point form for use by people with little or no coding experience.

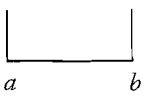
The Gaussian method of numerical integration has the disadvantage that the points at which the integrand must be evaluated are not equally spaced. If the integrand is a function that can be calculated at any point within the range of the integration, this is not a disadvantage for the Oracle. Another shortcoming of the Gaussian method is the cumbersome method of increasing the number of points at which the integrand is calculated in order to increase the accuracy. It was therefore decided to fix the code to do a

16-point Gaussian integration and to incorporate a method of dividing one integral into a sum of smaller integrals without leaving the subroutine, thereby replacing $\int_a^b f(x)\,dx$ by

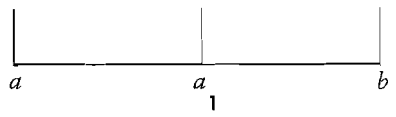
$$\int_a^{a_1} f(x)\,dx + \int_{a_1}^{a_2} f(x)\,dx + \ldots \int_{a_n}^{b} f(x)\,dx \quad .$$

In order to do this, a counter, called n^*, is included with the information given to the subroutine. This n^* is the number of times the interval (a to b) will be halved.

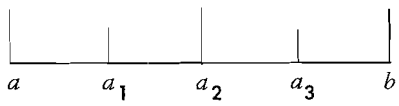
Therefore,

if $n = 0$, 

, $\int_a^b f(x)\,dx$;

if $n = 1$, 

, $\int_a^{a_1} f(x)\,dx + \int_{a_1}^{b} f(x)\,dx$;

if $n = 2$, 

,

$$\int_a^{a_1} f(x)\,dx + \int_{a_1}^{a_2} f(x)\,dx + \int_{a_2}^{a_3} f(x)\,dx + \int_{a_3}^{b} f(x)\,dx$$

and so on.

Because of the possibility of an error due to roundoff in this halving process, there is a correction for the interval a_n to b. It should be pointed out here that in halving the interval in a Simpson's Rule type of integration many of the same points are being evaluated again, but, in the Gaussian method, because of the irrational nature of the points, the second calculation is almost entirely independent of the first. So far, the series of integration routines includes the Gaussian single, Gaussian double, Gaussian triple integration, and the Simpson's Rule single integration. The multiple Gaussian integration has an n^* associated with each integral, so that each integral may have the number of points considered necessary by the programmer. The Simpson's Rule also has a built-in loop to double the number of points used in the integration. A comparison of the two single-integration schemes shows them to be of about the same speed, point for point, but that, in general, the Gaussian has much more accuracy and will converge to the correct answer, while Simpson's Rule may, because of roundoff, not converge at all.

NUMERICAL SOLUTION OF A SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS

Participating Member of Panel: C. L. Gerberich

The development of the Mauchly Modified Heun method of numerical solution of ordinary differential equations (see following section) pointed out the usefulness of the subroutine technique in the solution of these equations. That particular program still had many shortcomings for a general-purpose program: (1) it was a fixed-point method,

(2) it became quite cumbersome to handle a system of equations, and (3) it was not so accurate as the Runge-Kutta method. Therefore a program is being coded that will be in floating-point form, use the Runge-Kutta method, and have an internal loop to handle as large a system as there is space in the memory. The program will still have the built-in feature of advancement from one specified point to another of the independent variable. It is possible to go between any two points of the independent variable by using any size interval. There is already a large demand for the use of such a program as soon as it goes into production.

NUMERICAL INTEGRATION OF AN ORDINARY DIFFERENTIAL EQUATION BY USE OF THE MAUCHLY MODIFIED HEUN METHOD

Participating Member of Panel: C. L. Gerberich

In order to develop any good subroutine library, a great deal of time is required for experimentation with untried techniques. One such experiment gave rise to the Mauchly Modified Heun method subroutine for numerical integration of ordinary differential equations. The first question was the advisability of the use of a subroutine to handle such a problem. It was found, in general, that the subroutine program is very useful. The present code has the one shortcoming of being written in fixed-point form, but in the near future it will be recoded for floating-point arithmetic.

The program operates very much like the integration routines written up elsewhere in this report. Before entering the subroutine, the following information is supplied: the initial conditions, the value of the independent variable at which the subroutine is to be left, the number of times the interval is to be subdivided, and the location of a subroutine to calculate the derivative. This method makes it easy to move from one value which is to be punched to the next, even though the interval size required for the accuracy wanted is much smaller. The second question answered by this code is the machine practicability of this improvement of the Heun method. The method was presented by J. W. Mauchly to a class on computer mathematics given at Temple University. If two evaluations of $dy/dx = D_y$ are to be made for each step, it is reasonable to ask whether the extremes of the interval h are the best possible choices. Let it be assumed, for convenience, that one evaluation is made at the beginning of the interval, as with the Heun method. Instead of making the second one at $x + h$, let it be made at $x + g$, where g is to be determined so as to take into account the third as well as the first two terms of the Taylor series. Let $k_1 = gD_y(x,y)$ and $k_2 = hD_y(x + g, y + k_1)$. Then it is desirable to find the three constants, A, B, and g, so that $\Delta y = Ak_1 + Bk_2 +$ terms in $(hD)^4$ and higher powers. Equating coefficients of $Ak_1 + Bk_2$ with the Taylor series for Δy, it is found that: $Ag + Bh = h$, $Bhg = h^2/2$, $Bhg^2/2 = h^3/6$, hence; $g = (2/3)h$, $B = 3/4$, $A = 3/8$.

A significant increase in the accuracy of the Heun method has been accomplished without adding a great deal to the computational work. Perhaps this method has been derived before; the literature has not been searched to see whether others have proposed this scheme. If the method is not new, the failure to utilize its high adaptability to machine calculations would appear to be strange.

INTERPOLATION AND NUMERICAL DIFFERENTIATION BY USE OF DIVIDED DIFFERENCES

Participating Member of Panel: C. L. Gerberich

A need arose for a program that would calculate the derivative at several points within a range of experimental data. During the programming it was found that the proposed program was similar to one which would interpolate the experimental data within this same range. Therefore the two programs were combined and require the following information: whether the derivatives or interpolations are desired, the number of experimental points, the experimental points themselves (x_i, y_i), the number of points at which information is wanted, and a list of these points. The interpolation part of the program uses Newton's formula for interpolation with divided differences. This can be written as

$$f(x) \leqq f(x_1) + \sum_{s=1}^{n-1} \phi_s(x)\,(x_1\, x_2\, x_3\, \ldots\, x_{s+1}) \;,$$

where $\phi_s(x) = (x - x_1)\,(x - x_2)\,\ldots\,(x - x_s)$, and $(x_1\, x_2\, x_3\, \ldots\, x_{s+1})$ is the divided difference. Differentiating one time with respect to x gives

$$f'(x) \leqq \sum_{s=1}^{n-1} \phi_s'(x)\,(x_1\, x_2\, \ldots\, x_{s+1}) \;.$$

At the present time this program is in the coding stage. It should be ready for production in a short time.

COMPLEX ARITHMETIC

Participating Member of Panel: C. L. Gerberich

A program which will handle addition, subtraction, multiplication, and division of numbers of the form $a + bi$ has been put into a production status. The code uses the same interpretive three-address code that is used by the three-address floating-point routines and the double-precision arithmetic program. The program has been used to calculate functions with complex arguments, and good machine results have been obtained.

DIFFERENCES

Participating Member of Panel: C. L. Gerberich

Background and Status. In an effort to study the use of differences in error analysis, a code to punch out differences was written. The code is supplied with the number of

points, the number of differences wanted, and a list of the $f(x_i)$'s. The code punches out first the list of functions, then the first difference, and then the second, third, etc., until all the differences wanted are punched out.

At the present time a code to do a similar operation but with divided differences is being prepared for the Oracle. This code will be in floating-point form, while the original difference code is in fixed-point form.

DOUBLE-PRECISION ARITHMETIC

Participating Member of Panel: C. L. Gerberich

Background and Status. A need for a program that would do all types of arithmetic operations with numbers containing more than the 40 bits of the Oracle registers became evident quite early. There have been several problems where double-precision arithmetic was needed, but the floating-point method was used instead, with disastrous results. At present there exists a program that will provide addition, subtraction, multiplication, and division and which will use two memory locations to represent one number. The program has been "debugged" on the Oracle, but at the present time there is no estimate of the operation time. The program uses the same three-address representation that is used in several of the floating-point programs and the complex arithmetic program.

EQUIVALUE LINES FOR A TWO-DIMENSIONAL MESH

Participating Member of Panel: C. L. Gerberich

Background and Status. In the past a number of problems have been done on the Oracle, and the output consisted of the values of the solution at the intersections of an $m \times n$ mesh. It was found that the quantity of such an output is hard to understand unless it is put in the form of a graph. In general, the best graph is a contour type showing where the function has one particular value. If many different values of the function are to be plotted, the preparation of the graph proves to be a very time-consuming project. A code was desired to aid in the plotting of these contours.

Such a code was written with the following specifications. It is assumed that the function is already in the fast memory of the Oracle. The routine then requires the number of rows, the number of columns (these may be different), the number of different contours wanted, the location of the first value of the function in the memory, and a list of the values of the function for which contours are wanted. The code then punches an identifying word ($FFFFFFFFFF$) and the value of the function on the first contour. The code then systematically checks the mesh, row by row, until it finds two consecutive points of the mesh at which the values of the function lie on opposite sides of the contour value. It then calculates, by linear interpolation, the coordinates of the point at which this contour would cross the mesh line connecting these points. The code then punches the point ($F00 \ldots i0 \ldots j$) to mark the mesh point at which this happened. This is followed by the punch-out of the fractional part of the distance to point $(i + 1, j)$ at which the contour cuts the mesh.

The F punched in the ij word means that the following fractional part is to be added to the i component. After going row by row through the mesh, the program returns and goes column by column, the only difference being in the punching of the ij word. It now punches (0 . . . iF000 . . . j) and then the fractional part. This F shows that the fractional part is to be added to the jth component. When the code has finished this column-by-column search through the mesh, it will punch another identifying word (F . . . F) which means that a new contour is starting. This will continue until all the contours are finished.

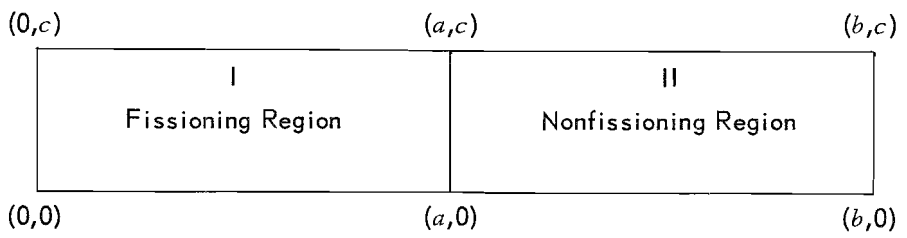
This method will give the approximate points at which the contour lines cut the mesh lines. The code has been used on several of the functions calculated in a one-group, one-region, two-dimensional bare reactor calculation. It was found that graphing of the results was considerably faster when this output was used. Future plans for this code include recoding for use with the anticipated photographic output of the Oracle. This enables the data to be used to plot the contours and to have them photographed.

Other codes for floating-point numbers and for three-dimensional meshes will be coded as needed.

TWO-DIMENSIONAL, TWO-REGION REACTOR CALCULATION

Participating Members of Panel: J. H. Alexander, C. L. Bradshaw, N. D. Given, W. R. Mann, W. C. Sangren

Background and Status. Investigations are being made concerning the two-dimensional, two-region reactor problem. As a first approach, the geometry and the analytic description of the flux are taken as indicated in the following diagram and in



the following material. The differential equation is

$$(\phi_{xx} + \phi_{yy}) - \frac{\Sigma_a \phi}{D} + \frac{S}{D} = 0 \ . \tag{1}$$

The boundary conditions are:

$$\phi(0,y) = \phi(b,y) = \phi(x,0) = \phi(x,c) = 0 \ , \tag{2}$$

where the flux is zero at the exterior boundaries;

$$D_1 \phi_{1_x}(a,y) = D_2 \phi_{2_x}(a,y) \ , \tag{3}$$

where the net neutron current is continuous across the core-reflector interface, and the

subscripts 1 and 2 refer to regions I and II;

(4) $$\phi_1(a,y) = \phi_2(a,y) \ ,$$

where the flux is continuous across the core-reflector interface.

This model readily lends itself to analytic solution, and three methods of solution have been explored. The results have been compared in order to determine the effectiveness of a numerical solution of more complicated models. The methods are as follows:

1. *Analytic solution of the differential system.* – The two differential equations,

$$\phi_{xx} + \phi_{yy} + B^2\phi = 0 \qquad \begin{cases} 0 < x < a \\ 0 < y < c \end{cases} \text{ with } B^2 = \frac{\nu\Sigma_f - \Sigma_a}{D} \ ,$$

$$\phi_{xx} + \phi_{yy} - K^2\phi = 0 \qquad \begin{cases} a < x < b \\ 0 < y < c \end{cases} \text{ with } K^2 = \frac{\Sigma_a}{D} \ ,$$

and the boundary conditions indicated above yield, as a solution, the transcendental equation

$$\tan ax + Lx = 0 \ ,$$

where

$$x = \sqrt{B^2 - \frac{\pi^2}{b^2}} \text{ and } L = \frac{D_1 \tanh\sqrt{K^2 + \frac{\pi^2}{b^2}}\,(b - a)}{D_2\sqrt{K^2 + \frac{\pi^2}{b^2}}} \ .$$

2. *Analytic solution of approximating difference system.* – If the derivatives in Eq. 1 are approximated by the relations

$$\phi_{xx} \approx \frac{\phi(x + h,y) - \phi(x,y) + \phi(x - h,y)}{h^2}$$

and

$$\phi_{yy} \approx \frac{\phi(x,y + h) - 2\phi(x,y) + \phi(x,y - h)}{h^2} \ ,$$

the solution to the resulting difference equation can be shown to be

$$\tan ax' + L' \sin(hx') = 0 \ .$$

The prime terms have indicated functions analogous to those in the solution of the differential system. In particular,

$$x' = \cos^{-1}\left(\frac{2 - \frac{h^2B'^2}{2} - \cos h\pi}{h}\right) \ ,$$

$$L' = \frac{D_1 \tanh (b - a)\gamma'}{D_2 \sinh (b\gamma')} ,$$

where

$$\gamma' = \frac{1}{b} \cosh^{-1} \left[2 + \frac{(bK)^2}{2} - \cos (b\pi) \right] ,$$

b = mesh size.

3. *Numerical solution of approximating difference system.* – Using the approximation for the derivatives, ϕ_{xx} and ϕ_{yy}, indicated in method 2, values of ϕ at various mesh points are given by the following equations:

$$\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j-1} + \phi_{i,j+1} - 4\phi_{i,j} + B^2 b^2 \phi_{ij} = 0 \tag{5}$$

for points in the fissionable region except on boundaries;

$$\frac{2D_2}{D_1 + D_2} \phi_{i+1,j} + \frac{2D_1}{D_1 + D_2} \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} - \frac{D_2 K^2 b^2}{D_1 + D_2} \phi_{i,j} - 4\phi_{i,j} + \frac{D_1 B^2 b^2}{D_1 + D_2} \phi_{i,j} = 0 \tag{6}$$

for points on the interior boundary;

$$\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} - 4\phi_{i,j} - K^2 b^2 \phi_{i,j} = 0 \tag{7}$$

for points in the nonfissioning regions.

The three methods described above have been coded for solution on the Oracle. The transcendental equations of methods 1 and 2 have been solved for various values of the parameters and for a mesh in the order of 20 × 20. The resulting values of B^2 have been compared, and the differences are well within the bounds expected. The resulting B'^2 of method 2 always lies somewhat below the B^2 of method 1.

The numerical solution of the approximating difference system requires the solution of a system of the type

$$A\Phi + B^2 M\Phi = 0 , \tag{8}$$

where A is a matrix of order $(b - 1)^2 \times (b - 1)^2$ and M is a diagonal matrix. The iteration scheme carried through for the system (8) is as follows:

(*a*) A vector $D^{(0)} = B^2 M\Phi$ is assumed.

(*b*) The resulting system $A\Phi^{(1)} + D^{(0)} = 0$ is solved by a successive iteration.

(*c*) B^2 is computed as $\Sigma D^{(0)}/\Sigma M\Phi^{(1)} \approx B^2$.

(*d*) $D^{(1)}$ is computed from the relation $D^{(1)} = B^2 M\Phi^{(1)}$.

The method has been run successfully on the Oracle for several parameter variations. A great deal of effort has been put forth in determining methods for increasing convergence in the solution of the system

$$A\Phi + D = 0 .$$

As indicated earlier, the method is to be applied to more complicated geometries, and, in addition, a more refined approximation to the derivatives ϕ_{xx} and ϕ_{yy} is to be investigated.

THE MEMBRANE PROBLEM

Participating Members of Panel: J. H. Alexander, C. L. Gerberich, W. C. Sangren

Background and Status. A general routine for calculating the fundamental eigenvalue and eigenfunction associated with a membrane having fixed boundaries in the xy plane has been coded and run on the Oracle. The eigenfunction is computed on a square mesh, and the boundaries are assumed to lie on the straight lines between these mesh points. It is possible to make either the function or its derivative equal to zero on the boundary. This is, therefore, a one-region or bare reactor type of calculation. About 80 cases have been carried out with this code.

Most of the cases which have been run are for the square or L-shaped regions. A few cases of T's, crosses, and square doughnuts have also been run. A large number of squares were run because not only is the solution to the differential system known but also the solution to the difference system which the machine is trying to solve. For certain convex regions, Forsythe has proved that the fundamental eigenvalue associated with the difference equations is a lower bound. With the customary difference operator, A, for the square, the convergence of the power method is very poor, since even after 200 iterations the machine result for the eigenvalue is larger than the analytical eigenvalue. Even iterating the best linear function of A gives unsatisfactory results. After much experimentation it was verified that a method presented in a paper by Flanders and Shortley leads to favorable results. In this method the iteration is carried out by using an appropriate Chebychev polynomial of the operator A, and it was possible to obtain the eigenvalue for the difference system, accurate to eight significant figures after 60 iterations.

The only difficulty with the Chebychev polynomial method is that, for good results, it is necessary to know about where the fundamental eigenvalue is located and that the second eigenvalue is separated sufficiently from this location. In the case of odd-shaped domains, this information is not available in advance. An estimate for the first two eigenvalues can be obtained from the results of about 20 iterations with the operator A plus an intelligent guess.

Two types of calculations have been carried out for symmetric L-shaped regions. A symmetric L consists of a square with a smaller square cut out of one corner. The

boundary is assumed to have a zero value for the function. In the first type of calculation the size of the smaller square is varied, and in the second type the smaller square is kept fixed but the mesh size is varied.

For calculations of the first type, the basic square consists of size 25 by 25, where the distance between neighboring mesh points is taken to be 1. For the second type, the distance between mesh points is again taken to be 1 and the size of the similarly shaped L's is determined by the number of mesh points. The L was chosen because it is a nontrivial region where an investigation of shape and mesh size might clarify the procedures to be used on more complicated shapes.

Two additional codes were written and used in connection with these calculations. The previously mentioned general routine or code is an iterative method based upon the difference equations which approximate the differential equations. By using the eigenfunction obtained by the iterative method, it is possible to find an upper bound for the eigenvalue by calculating the ratio of two integrals which appear in the associated variational problem. One of the additional codes, therefore, consists in using an appropriate integration scheme and finding this upper bound for the eigenvalue. The remaining code also deals only with the processing of the final iterated eigenfunction. The eigenfunction is calculated at the mesh points. This is not, in general, the information that is easily comprehended. The most easily understood representation consists of level lines or lines of constant values. This code essentially obtains these level lines. It is described elsewhere in this report.

COMPLEX FUNCTION SUBROUTINES

Participating Members of Panel: S. E. Atta, S. G. Campbell

Background and Status. The appearance of complex-valued functions of complex variables in the M-shell internal conversion problem has pointed out the necessity of having available such functions as standard Oracle subroutines. Accordingly, subroutines have been written for calculating ln z, sin z, cos z, and z^w (where both z and w may be complex numbers). These codes are now being tested on the Oracle and will be available in standard subroutine form as soon as testing is complete. Several possible numerical methods are also being tested in the evaluation of the complex Γ function.

SUBROUTINES FOR ELEMENTARY FUNCTIONS

Participating Member of Panel: M. R. Arnette

Status. Two more subroutines for computing elementary functions for use with floating-point operations, Subroutine Library (SRL) No. 3.1b, have been checked out; SRL No. 3.1b is the floating-point arithmetic with a number of the form $x = a \cdot 2^b$ filling one word. Thirty bits are used for a and ten bits for b, with $\frac{1}{2} \leqq |a| < 1$, $|b| \leqq 511$. The code fills 91 words, has one entry, and has eight order commands. The two added

functions are $y = e^x$ and $y = \ln x$. Also, there is a conversion routine now which takes input numbers in the form $q = d \cdot 10^p$, where d is a decimal $\geqq 0.1$ and <1.0 in magnitude, p is a decimal integer $\geqq 0$ and $<10^9$ in magnitude. These input numbers are converted by the routine to a (30-10) machine number, that is, to $a \cdot 2^b$, where $\frac{1}{2} \leqq |a| < 1$ is the first 30 bits and b is the last 10 bits.

Four more continued fractions subroutines for fixed-point arithmetic have been added:

1. $y = \tanh x$,
2. $y = e^x$, $x < 0$,
   $y = \frac{1}{4} e^x$, $x \geqq 0$,
3. $y = 2^{-1} \tan x$,
4. exponential and hyperbolic functions, $-1 \leqq x < 1$.

An additional code for matrices has been written.

Suppose that by some process of operating upon y in the system $Ax = y$ an x_0 has been obtained which, however, is not exact because of propagated or generated error. This code will get a better x by means of an iterative process. If $A = n \times n$, then n must be less than or equal to 28.

CALCULATION OF HIGHER MATHEMATICAL FUNCTIONS BY NUMERICAL QUADRATURE

Participating Member of Panel: S. G. Campbell

Background and Status. Use was made of the fact that, for certain classes of functions (including the Bessel I, J, H, and K functions), the trapezoidal rule is a highly accurate numerical quadrature formula and is, in particular, much more accurate than Simpson's Rule for the same number of points. Since these functions lack a simple addition formula and also generally require two different series expansions for different ranges of the argument, numerical quadrature by means of the trapezoidal rule was used to construct a single, short code which would handle any desired range of the argument for the Bessel functions J_n and I_n, with integral n and either real or complex argument. The procedure is now being tested on the Bessel functions, H_n and K_n, in addition to various other of the higher transcendental functions which have usable integral representations. A subroutine to calculate $\ln (1 + x)$, $0 \leqq x < 1$, has also been tested by using Gaussian numerical integration. It is of comparable accuracy with the existing subroutine which calculates $\ln (1 + x)$ as a continued fraction on the same range and is 10 msec faster than the continued-fraction subroutine. The same technique is being tested as a possible means of calculating the probability integral with a high degree of speed and accuracy.

CALCULATION OF THE GENERALIZED HYPERGEOMETRIC SERIES

Participating Member of Panel: S. E. Atta

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Status. A ${}_pF_q$ program for complex parameters and complex argument has been written as a subroutine for the Oracle by using floating-point operations. This subroutine will take any number of p's and q's.

A THREE-ADDRESS FLOATING-POINT SYSTEM FOR THE ORACLE

Participating Members of Panel: S. G. Campbell, C. P. Hubbard, M. F. Todd

Background and Status. A complete, new floating-point system has been programmed for the Oracle by using three-address interpretive commands. Each command consists of one word or ten hex digits – three addresses of three digits each and one digit to specify the operation. Initial entry into the floating-point routine requires only one word, and exit from the floating-point routine is automatic on a breakpoint address. The advantages of the three-address system are that coding is extremely simple and straightforward and that, in general, a program using this system will be shorter than one using any other type of floating point. Two codes are available; in one the magnitude and exponent of a number are packed in a single word, while in the other, two words are required for each number. In addition to the floating-point code, the system includes full decimal input and output conversions, an exponential subroutine, and a square-root subroutine. The exponential routine uses the expansion of e^x as a continued fraction. The calculation of e^x in this manner is much faster than the calculation in which the power series for e^x is used.

A BINARY FLOATING-POINT SUBROUTINE

Participating Member of Panel: S. E. Atta

Background and Status. The binary floating-point subroutine is comparatively shorter than any of the other existing Oracle floating-point subroutines and is comparable in computation time; it is also easy to use. A separate entrance position for multiplication, division, and addition is an aid to decreasing the computation time. The main routine requires, for each floating-point operation, two consecutive words. The first word is a code written in the same manner as that used for fixed-point computations. However, this word consists of the operation to be performed and the memory positions of the two numbers to be operated upon. The second word is a code for the storage position of the result and entrance to the next floating-point operation or an exit from floating-point to the main routine. Two consecutive memory positions are required for each number and its exponent. The routine has been used in several problems and subroutines.

NONLINEAR SYSTEMS OF EQUATIONS

Participating Members of Panel: R. C. F. Bartels, A. C. Downing

Background and Status. Only two or three general methods are known for numerically treating nonlinear systems of equations. The method of steepest descent is one of these. Although it applies specifically to the location of a relative maximum or minimum of a function of n real variables, it is clear that any solution of an arbitrary nonlinear system

$$\phi_i(x_1, \ldots, x_n) = 0 , \qquad i = 1, \ldots, n ,$$

will be a minimum of the quadratic form

$$Q = \sum_{i,j=1}^{n} a_{ij}\phi_i\phi_j ,$$

where the a_{ij} are the elements of some positive definite matrix. A frequent choice for this matrix is the identity matrix, in which case

$$Q = \phi_1^2 + \phi_2^2 + \ldots + \phi_n^2 .$$

A general program has been prepared for the Oracle; this program uses the method of steepest descent to find extreme values of any desired function $Q(x_1, x_2, \ldots, x_n)$ of n variables. The particular function is inserted into the program in the form of a subroutine. The process is iterative. For each iteration, the steepest descent program computes the direction of the gradient of the function at some previously determined point. In order to estimate the location of the extremum in the gradient direction (that is, in the direction of steepest descent), the value of the function is computed at three points in this direction, and these points are fitted to a parabola with a vertical axis. The location of the vertex of this parabola is the new estimate for the extremum point. That is, Newton's method is applied to the derivative of a plane curve lying on the surface $y = Q(x_1, \ldots, x_n)$ and passing through the specified point in the direction of the gradient.

This process converges provided the initial approximation is sufficiently good. Just what this means depends very strongly upon the particular problem.

An earlier program, which is a modification of the method of steepest descent, was written for the Oracle. Instead of moving in the gradient direction, the successive new estimates were obtained by applying Newton's method to the derivative of a curve lying in one of the coordinate planes. The n coordinate planes were used in cyclic succession. This method was discarded after it was discovered that it is easy to devise functions for which the method would converge very slowly. Consider, for example, a surface with a long, narrow channel leading down to the minimum. If the projection of this channel is not parallel to one of the coordinate axes, then the process of successive minimizations in the coordinate directions will progress very slowly to the

desired minimum. Such channels also cause trouble in the true steepest descent process because the direction of the gradient changes rapidly as the distance from the center of the channel is increased.

INVERSE CHARACTERISTIC VALUE PROBLEM

Participating Members of Panel: R. C. F. Bartels, A. C. Downing

Background and Status. The following problem is of interest in the analytical treatment of certain dynamical systems: given the $n \times n$ symmetric matrix G, determine the diagonal matrix F such that the determinant $|G - \lambda F|$ vanishes for a given set of real numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$. It is easily seen that in the special case $n = 2$ a solution need not exist even for the case in which G is positive definite, or if a solution does exist it need not be unique. The criteria for the existence and the uniqueness of a solution in the general case do not appear to be known. However, in certain special cases physical evidence might be sufficient to indicate that at least one solution can exist.

A solution has been obtained for a special case in which $n = 5$. A combination of two numerical techniques was used in arriving at this solution. One method based on the principle of steepest descent was used in an attempt to determine the elements f_K (where $K = 1, 2, 3, 4, 5$) of the diagonal matrix F for a given set of values λ_K (where $K = 1, 2, 3, 4, 5$). This method exploits the fact that the positive definite function of the elements of the matrix F, namely,

$$Q = \sum_{K=1}^{5} |G - \lambda_K F|^2 ,$$

vanishes for any set of values of f_K representing a solution of the problem and, therefore, that it has a minimum for these values of f_K. Starting with an initial estimate, successive approximations of the values of f_K which minimize Q are obtained by Newton's method. Each step of this iterative process is taken in the direction of the gradient of the function Q and, therefore, in the direction of most rapid variation of Q. This method meets with some success. That is, successive estimates are improvements, but the convergence is extremely slow, except when the initial estimate of the elements of F is very close to the required minimum.

The second method is based upon the observation that approximate values of the elements of the matrix F can, in certain cases, be improved by following iterative procedure. If $f_K^{(n)}$ (where $K = 1, 2, \ldots$) denote the values of the elements of the diagonal matrix F_n at any step in this process, then an improved set of values is given by

$$f_K^{(n+1)} = \frac{\lambda_K^{(n)}}{\lambda_K} f_K^{(n)} , \qquad (K = 1, 2, \ldots) ,$$

where λ_K (where $K = 1, 2, \ldots$) are the given values and $\lambda_K^{(n)}$ (where $K = 1, 2, \ldots$) are the zeros of the determinant $|G - \lambda F_n|$, the λ's and the f's having an appropriate order. It is assumed, of course, that $\lambda_K \neq 0$ and, therefore, that the required matrix F is positive definite. It should be observed that the numbers λ_K and $\lambda_K^{(n)}$ are the characteristic values of the symmetric matrices $F^{-1/2}GF^{-1/2}$ and $F_n^{-1/2}GF_n^{-1/2}$, respectively. It should also be observed that the values of the elements $f_K^{(n+1)}$ which are defined at each step of this process are such that the product of the characteristic values $\lambda_K^{(n+1)}$ is equal to the product of the given λ_K. Hence the process preserves one of the invariants of the matrix $F^{-1/2}GF^{-1/2}$.

After the solution was obtained, additional calculations were carried out, and these indicate that, in the special case treated, the second method would have been sufficient to determine the solution. However, because of the large amount of coupling between three of the elements of F, it is not obvious that this method should converge in the large for this special case.

PROBLEMS

A TEST FOR RANDOM FUSION OF ISOCHROMATID BREAKS IN *TRADESCANTIA*

Origin: A. D. Conger, Biology Division

Participating Members of Panel: A. W. Kimball, G. J. Atta

Background and Status. An isochromatid break in *Tradescantia* occurs when two sister chromatids are broken at the same place. The broken ends can rejoin or fuse in six different ways. If the chromatids rejoin as they were before breakage or if the two sister chromatids simply exchange distal ends, no real genetic change results and restitution is said to have occurred. If the two proximal ends rejoin and the two distal ends rejoin, the result is observable phenotypically. All three of these types of rejoining require two fusions. It is possible that only one fusion will occur, and this can take place between either the proximal or the distal pair of broken ends. Finally, neither pair of broken ends may fuse.

The two types of rejoining which result in restitution are never observed, since these cells cannot be distinguished genetically from normal cells. The remaining four types of rejoining result in aberrations and can be identified separately. In Table 1, the probabilities, observed frequencies, and expected frequencies for five classes are given for the hypothesis of random fusion. The two types of rejoining which result in restitution have been pooled to make up the first (unobservable) class, and p is the probability of single fusion. On the basis of previous evidence it has been assumed that restitutions occur with the same frequency as that for two-fusion aberrations.

TABLE 1. FREQUENCIES OF TYPES OF REJOINING

Type of Rejoining	Probability	Observed Frequency	Expected Frequency
Restitution	$\theta_1 = p^2/2$	(T_1)	$N\theta_1$
Two-fusion aberration	$\theta_2 = p^2/2$	T_2	$N\theta_2$
One-fusion aberration (distal)	$\theta_3 = p(1-p)$	T_3	$N\theta_3$
One-fusion aberration (proximal)	$\theta_4 = p(1-p)$	T_4	$N\theta_4$
No-fusion aberration	$\theta_5 = (1-p)^2$	T_5	$N\theta_5$
Total	1	(N)	N

If T_1 could be observed, a test of the random-fusion hypothesis could be made by the conventional chi-square method. Since this class is not observed, two parameters, p and T_1 (or N), must be estimated from the data. The minimum chi-square method of estimation proved to be the simplest to apply. The quantity to be minimized with respect to p and T_1 is

$$X^2 = \sum_1^5 \frac{(T_i - N\theta_i)^2}{N\theta_i} .$$

It may be shown that

$$\frac{\partial X^2}{\partial T_1} = \frac{1}{\theta_1}\left(\frac{2NT_1 - T_1^2}{N^2}\right) + (\theta_1 - 2) - \frac{1}{N^2}\sum_2^5 \frac{T_i^2}{\theta_i} + \sum_2^5 \theta_i ,$$

and if this is set equal to zero and solved for N, the result is

$$N = \left(\frac{A^2 + \theta_1 \sum_2^5 \frac{T_i^2}{\theta_i}}{1 - \theta_1}\right)^{1/2} ,$$

where $A = \sum_2^5 T_i$. A good initial estimate for p is

$$p_0 = \frac{2T_2 + T_3 + T_4}{2A} .$$

The quantity N may be computed for various values of p in the vicinity of p_0, and for each pair of (N,p) values, chi-square may be computed and plotted against p. Thus the minimum chi-square estimate of p (and hence N) may be obtained graphically. The minimum chi-square will have three degrees of freedom.

In one experiment, $T_2 = 2054$, $T_3 = 98$, $T_4 = 68$, and $T_5 = 33$. From these values, $p_0 = 0.948$. Chi-squares were computed for $p = p_0$, 0.94, 0.96, and 0.97, and the minimum chi-square of 187 was found at $p = 0.958$. For three degrees of freedom, this is highly significant, and the hypothesis of random fusion must be rejected.

SAMPLING METHODS FOR RADIOPROTECTION STUDIES WITH MICE

Origin: W. T. Burnett and D. G. Doherty, Biology Division

Participating Member of Panel: A. W. Kimball

Background and Status. Most of the studies with radioprotective compounds have dealt with bacteria and other small organisms. The list of such compounds is a lengthy one, and for such studies to be extended economically to higher forms of life, methods of sampling and testing had to be found which would provide the maximum amount of information with the fewest possible animals. For each compound, the experimental work consists of two phases. In the first phase the toxicity of the compound is investigated, and this determines suitable dose levels of the compound for use in the second phase in which radiation protection is studied.

The sampling method employed in the toxicity phase is known as the "up-and-down" method.[1] A set of doses, usually equally spaced on a log scale, is chosen a priori. One animal is injected at a dose believed to be near LD_{50}. If this animal dies, a second animal is injected with the next lowest dose; if the first animal lives, the second animal is injected with the next highest dose. The procedure is continued until a predetermined number of animals have been tested. It was found that LD_{50} could be estimated, usually, within 5%, with only ten animals tested. Other methods, such as probit analysis, of estimating LD_{50} could easily require 50 or more animals to achieve standard errors of 5% or less.

In the radiation phase, the method of sequential analysis[2] was used for testing the difference in six-day mortality between two groups of mice exposed to x radiation, one group having been pretreated with a compound, the other group serving as controls. In this type of experiment, the sample size is not fixed but, instead, depends on the outcome of the experiment. Each step in the experiment consists in the exposure of two subgroups of m animals each and a comparison of the accumulated mortalities in the two groups at the completion of each step. Let

E_i = number of animals living in the ith treated subgroup,

C_i = number of animals living in the ith control subgroup,

m = number of animals living per subgroup.

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[1] K. A. Brownlee, J. L. Hodges, Jr., and M. Rosenblatt, *J. Am. Stat. Assoc.* **48**, 262–277 (1953).

[2] A. Wald, *Sequential Analysis*, Wiley and Sons, New York, 1947.

Then at each step the quantities

$$y_i = E_i - \frac{E_i C_i}{m} \qquad \text{and} \qquad x_i = E_i + C_i - \frac{2E_i C_i}{m}$$

are computed. If k steps have been performed, the quantity $\sum_{i=1}^{k} y_i$ is compared with $\left(\pm a + b \sum_{i=1}^{k} x_i\right)$, where a and b are predetermined constants. The action to be taken is then determined as follows:

1. If $\sum_{i=1}^{k} y_i > a + b \sum_{i=1}^{k} x_i$, the experiment is stopped, and the compound is judged to be protective.

2. If $\sum_{i=1}^{k} y_i < -a + b \sum_{i=1}^{k} x_i$, the experiment is stopped and the compound is judged to be not protective.

3. If $-a + b \sum_{i=1}^{k} x_i < \sum_{i=1}^{k} y_i < a + b \sum_{i=1}^{k} x_i$, the experiment is continued.

In these experiments $b = \frac{1}{2}$, and in this case the inequalities in (1) and (2) reduce to

$$\sum_{i=1}^{k} (E_i - C_i) > 2a \qquad \text{and} \qquad \sum_{i=1}^{k} (E_i - C_i) < -2a ,$$

respectively. Thus the experiment is stopped whenever the number of animals living in the treated group either exceeds the number living in the control group by $2a$ or is less than the number in the control group by $2a$.

This type of experiment has two advantages which make it ideal for radioprotection studies with animals. It requires fewer animals, on the average, than any method of fixed sample size. The savings can be as much as 50%. Furthermore, it enables the experimenter to control both kinds of error. That is, he may judge a compound to be protective when actually it is not, or he may judge a compound to be not protective when actually it is. In sequential analysis it is possible to assign predetermined risks for both types of error, whereas in experiments of fixed sample size, only the first kind of error can be controlled.

POWER FUNCTION CALCULATIONS FOR A CHRONIC NEUTRON EXPERIMENT WITH MICE

Origin: A. C. Upton, Biology Division

Participating Members of Panel: A. W. Kimball, G. J. Atta

Background and Status. In a chronic neutron experiment now being planned with mice, incidences of cataracts, leukemias, and tumors will be studied. In each case a control group will be compared with an irradiated group. The observed frequencies for such a comparison may be represented as in Table 2, where n is the number of animals per group, p is the proportion of animals with tumors in the control group, and $\bar{p}$ is the proportion of animals with tumors in the irradiated group. The null hypothesis, $E(p) = E(\bar{p})$, will be tested at the $\alpha = 2.5\%$ level by means of a chi-square with one degree of freedom.

TABLE 2. OBSERVED FREQUENCIES OF TUMORS

	With Tumor	Without Tumor	Total
Control group	np	$n(1-p)$	n
Irradiated group	$n\bar{p}$	$n(1-\bar{p})$	n
Total	$n(p+\bar{p})$	$n(2-p-\bar{p})$	$2n$

With the risk of the first kind of error (rejecting the null hypothesis when it is true) controlled at ±2.5%, the question arose as to the power of the test (one minus the probability of accepting the hypothesis when it is false) for various values of n and $E(p - \bar{p})$. From Table 2, the chi-square is

$$X^2 = \frac{2n(\bar{p} - p)^2}{(p + \bar{p})(2 - p - \bar{p})},$$

and for large n, X is distributed approximately as a normal deviate with zero mean and unit variance. Thus tables of the power function for normally distributed variates may be used to approximate the power of the test to be used in this experiment. These calculations were performed with the aid of data from a previously published table.[3] The normal incidence of leukemia was substituted for $E(p)$, and the power of the test was computed for $n = 100(50)250$ and $E(\bar{p}) = 0.03(0.01)0.10$, 0.15, and 0.20.

[3] E. S. Pearson and H. O. Hartley (ed.), *Biometrika Tables for Statisticians*, Vol. 1, Table 10, Cambridge University Press, 1954.

A TEST FOR POSITION EFFECT IN A CYCLOTRON EXPERIMENT

Origin: F. P. Conte and A. C. Upton, Biology Division

Participating Members of Panel: A. W. Kimball, G. J. Atta

Background and Status. Neutron experiments with mice in the 86-in. cyclotron have been described previously.[4] The animals are irradiated within a lead chamber and are held in widely separated positions by means of Lucite stanchions. A photograph of this exposure device has already been issued.[5]

One of these experiments was a dose fractionation study in which three groups of mice received total doses in two halves, separated by intervals of 2, 5, and 8 days, respectively. A fourth group received total doses in single exposures and served as a control group. Six of the nine positions in the Lucite stanchions were used for this experiment so that each group consisted of six subgroups, each receiving a different total dose. The mortality data were subjected to the angular transformation, and the transformed data were plotted linearly against dose. It was observed, however, that negative and positive deviations from regression seemed to be correlated with position. That is, if a particular dose point fell below the fitted curve in one group, it was likely to fall below the fitted curve in the other three groups, and similarly for positive deviations. This suggested a position effect, in the exposure box, which could be interpreted as errors in dosimetry. The fact that this effect formed a pattern in the box with respect to the location of the target lends added strength to the hypothesis. In the final analysis of the experiment it was necessary to evaluate the position effect, test for its significance, and make whatever corrections were possible.

Since the dose and position effects were completely confounded, it was impossible to correct the LD_{50} estimates for bias because of the position effect. Fortunately, the differences in LD_{50} estimates were not biased, so that comparisons among the four groups were valid. It was possible, however, to evaluate the position effect and to remove this added component of variation from the residual variance. This is shown in Table 3. If there were no position effect, mean square (A) would be about equal to mean square (B), and there would be 16 degrees of freedom for estimating the residual variance. A variance ratio test showed that (A) was significantly greater than (B) at the 4% level. Thus the position effect was established, and this source of variation was removed from the residual variance, leaving 12 degrees of freedom. The remaining tests of significance and confidence intervals were computed with the reduced residual variance.

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[4] A. C. Upton *et al.*, *Biol. Semiann. Prog. Rep. Aug. 15, 1954*, ORNL-1766, p 55.

[5] *Ibid.*, Fig. 24, p 57.

TABLE 3. ANALYSIS OF VARIANCE (ANGULAR UNITS)

Source of Variation	Degrees of Freedom	Mean Square	Variance Ratio	Level of Significance (%)
Average regression	1	1.0706		
Deviations from average regression	4	0.0927 (A)	3.52	4.0
Among groups	3	0.1802	6.85	0.6
Slope × group interaction	3	0.0499	1.90	19.0
Residual variance	12	0.0263 (B)		
Total	23			

INTERPRETATION OF EXPERIMENTS ON THE CONTROL OF NUCLEAR RATIOS IN *NEUROSPORA* HETEROKARYONS

Origin: T. H. Pittenger and K. C. Atwood, Biology Division

Participating Members of Panel: A. W. Kimball, G. J. Atta

Background and Status. For certain experimental work with *Neurospora* heterokaryons, it is desirable to be able to control the nuclear ratio. If heterokaryons are formed from two biochemical mutants, say A and B, and if these are mixed in a predetermined nuclear ratio, it would be advantageous if the resulting population of conidia maintained the initial ratio. In practice the initial ratio is not maintained, but the final ratio is related to the initial ratio in a regular, reproducible manner which suggests certain interpretations. One of these interpretations is that the two types of nuclei divide at different rates, and an attempt was made to test this hypothesis.

Let x_a and x_b be the initial numbers (unknown) of the two types of nuclei. These are mixed together in a series of known proportions, $x_a/(x_a + x_b)$, usually ranging from 0.10 to 0.90. Further, let the division rates be such that after a fixed length of time, there are $\lambda_a x_a$ and $\lambda_b x_b$ of the two types of nuclei present. At this point the conidia are sampled, and the proportions $\lambda_a x_a/(\lambda_a x_a + \lambda_b x_b)$ are determined. Now let

$$X = \frac{x_a + x_b}{x_a} - 1 \qquad \text{and} \qquad Y = \frac{\lambda_a x_a + \lambda_b x_b}{\lambda_a x_a} - 1 .$$

Then $Y = (\lambda_b/\lambda_a)X$. If the model is correct, the function Y should plot linearly against the function X. If there is no difference in division rates, the slope should be 1.

When this method was applied to data from several experiments representing different heterokaryons, slopes differing significantly from 1 were found in every case, but the plots were not quite linear. However, the plot of Y against X^n was linear for values of n between 0.7 and 0.8. This indicates that some modification of the original hypothesis is necessary before an adequate explanation can be found.

A RATE PROBLEM IN *DROSOPHILA* GENETICS

Origin: W. K. Baker, Biology Division

Participating Member of Panel: A. W. Kimball

Background and Status. The number of a certain type of progeny in the nth generation from a genetic cross in *Drosophila* is given by

$$g(p,n) = \frac{p^n}{2 - p^n}, \qquad 0 \leqq p \leqq 1 .$$

The question is whether the relative rate of change of $g(p,n)$ with respect to p increases from generation to generation. The quantity in question is

$$\frac{\partial g(p,n)}{\partial p} \cdot \frac{1}{g(p,n)} = \frac{2n}{p(2 - p^n)} = h(p,n) ,$$

and the inequality to be proved is $h(p,n + 1) > h(p,n)$ for all n and p. This may be written

$$\frac{2(n + 1)}{p(2 - p^{n+1})} > \frac{2n}{p(2 - p^n)} ,$$

or, alternatively,

$$p^n[n(1 - p) + 1] < 2 . \tag{1}$$

Let $f(n) = p^n[n(1 - p) + 1]$ and $R = f(n + 1)/f(n)$. The inequality $R \leqq 1$ will be satisfied if

$$p[(1 - p)(n + 1) + 1] \leqq (1 - p)n + 1 .$$

But this reduces to

$$(1 - p)^2 (n + 1) \geqq 0 ,$$

and it is clear that this relationship holds for all admissible n and p. Hence $R \leqq 1$, or $f(n + 1) \leqq f(n)$. Furthermore, $f(0) = 1$, so that inequality (1) is clearly satisfied for all n and p.

CURVE-FITTING OF THE INTEGRATED MICHAELIS-MENTEN EQUATION

Origin: D. G. Doherty, Biology Division

Participating Member of Panel: A. W. Kimball

Background and Status. Many different attempts have been made to fit experimental data to the integrated form of the Michaelis-Menten equation

$$-\frac{dS}{dt} = \frac{VS}{k + S} , \tag{1}$$

where S is the amount of substrate present at time t, V is the maximal velocity, and k is the reciprocal of the Michaelis constant. A recent discussion of this problem is given by Fleisher.[6] For certain reactions, none of these methods seems to provide very good

[6] G. A. Fleisher, *J. Am. Chem. Soc.* **75**, 4487 (1953).

estimates. In such cases, the method of multiple regression was found to work very well.

Integration of Eq. 1 yields

$$Vt = k \log \frac{S_0}{S} + (S_0 - S) , \tag{2}$$

where S_0 is the initial substrate concentration. For purposes of curve-fitting, it is convenient to let $x = S_0 - S$, the concentration of the product formed during time t. Then Eq. 2 can be written in the form

$$\log \left(\frac{S_0 - x}{S_0} \right) = \frac{1}{k}(x) - \frac{V}{k}(t) , \tag{3}$$

which can be fitted by means of multiple regression, with x and t serving as the independent variates. This method was found to provide estimates of k and V, with errors of 10% or less, when other methods failed.

URANIUM DISTRIBUTION AND EXCRETION STUDIES IN MAN

Origin: S. R. Bernard, Health Physics Division

Participating Members of Panel: J. Z. Hearon, A. S. Householder, A. W. Kimball, G. J. Atta

Background and Status. Consideration of the study of uranium distribution and excretion in man has been under way in the Health Physics Division for some time. The general problem is of considerable scope and complexity. Those phases with which this Panel is concerned will presumably constitute a continuing problem in the future. They are described here for purposes of reference and to delineate the current status.

The immediate purpose of the study is to provide a method which permits the amounts of uranium in the body tissues (and hence the internal radiation dose) to be inferred from measurements of urinary excretion of uranium. With such a method, it would be possible, by the relatively simple procedure of determining urinary uranium on routinely exposed production personnel, to compute internal radiation doses and to prescribe an internal-dose control program. Further, useful data could be furnished to the National Committee on Radiation Protection.

The problem centers about a model which relates the amount, x_i, of uranium in the ith body tissue or "compartment" to that in all other compartments:

$$\dot{x}_i = \sum_{j=1}^{n} k_{ij} x_j , \qquad i = 1, 2, \ldots , n , \tag{1}$$

where, in particular, x_n is the amount in the urine and $k_{nj} = 0$ for all $j \neq n - 1$, since there is no return from the urine to any other tissue. In general, the solution of

Eq. 1 is of the form

$$x_i = \sum_{j=1}^{n} a_{ij} e^{\lambda_j t} , \qquad i = 1, 2, \ldots , n , \tag{2}$$

where the λ_j are the roots of the matrix K, and $A = (a_{ij})$ is a matrix such that $AKA^{-1} = \Lambda = \text{diag}\,(\lambda_1, \lambda_2, \ldots , \lambda_n)$. It can be shown that $\lambda_i \leqq 0$ for all i and that at least one $\lambda_i = 0$ (ref. 7). Since $x_n(t)$ can be observed, a_{nj} and λ_j can be determined, in theory, by fitting Eq. 2 to the observed data. It is then possible to compute, from the characteristic equation and the relation $AKA^{-1} = \Lambda$, the k_{ij}. The problem thus consists of the fitting procedure, the description of the model, and the checking of the computed $x_i(t)$, $i < n$, against the observed $x_i(t)$, $i < n$.

Estimates of the a_{nj} and λ_j were attempted by Householder's modification of Prony's method.[8] The orthogonalization procedure for determining n, the number of exponentials and initial estimates, and the iterative procedure for improving estimates of the elementary symmetric functions of the $e^{\lambda_i b}$ have been coded for the Oracle by B. L. Harless. An actual set of data showed the orthogonalization procedure to be satisfactory, but the iteration converged on untenable results. A synthetic set of data [values of $x_n(t)$ computed from Eq. 2 with known a_{nj} and λ_j were assigned errors, Poisson distributed at three variance levels] was then processed. It was established that at zero or sufficiently low variance levels the iterative procedure converged upon satisfactory results. However, at variance levels of the order which would be encountered in actual problems the results were not satisfactory. The orthogonalization procedure has been retained and recoded for the general case. Estimates of the a_{nj} and λ_j were attempted by the procedure of Deming.[9] This procedure proved to be unsatisfactory, and a comparative study of the Deming and the Garwood[10] methods indicated that in the Deming method the matrix of normal equations is "nearly singular" (due to the fact that the derivatives of the sum of squares of deviation with respect to the λ_i are very highly correlated) but that this difficulty does not occur in the Garwood method. Application of the Garwood method and a comparative study of this method and the straightforward solution of the nonlinear normal equation are being made.

An adequate model for lung–lymph-node interchange following long-term exposure to insoluble uranium-containing dust particles has been obtained and is to be applied to data collected by the Rochester group. The deduction of the k_{ij} has been achieved for $n \leqq 4$. This is, in general, not a trivial problem, and new methods have been devised

[7] J. Z. Hearon, *Bull. Math. Biophys.* **15**, 121 (1953).

[8] A. S. Householder, *On Prony's Method of Fitting Exponential Decay Curves and Multiple-Hit Survival Curves*, ORNL-455 (Sept. 19, 1949).

[9] W. E. Deming, *Statistical Adjustment of Data*, Wiley and Sons, New York, 1943.

[10] F. Garwood, *Biometrika* **32**, 46 (1941).

which promise to suffice for general n, provided some restriction upon the connectivity of the compartments can be imposed. Final decisions along these lines await comparison of observed and computed $x_i(t)$, $i < n$. Observed values are being obtained from human subjects in a cooperative project between the Health Physics Division and W. H. Sweet, Massachusetts General Hospital.

COMPUTATION OF H_2O_2 IN MICRONUCLEUS OF *PARAMECIUM*

Origin: R. F. Kimball, Biology Division

Participating Members of Panel: J. Z. Hearon, N. M. Dismuke

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Background and Status. Rough calculations have previously been made of the mean concentration of H_2O_2 inside a cell during and after irradiation. The original equations (above reference) were approximate in that (1) an approximate version of the diffusion equation was used and (2) certain rapid transients were neglected for preliminary purposes. The error in the approximate diffusion equation[11,12] can be assessed, and from observed consumption rates of H_2O_2 by the cells it can be shown that an error of $\leqq 20\%$ is entailed in assuming that "the concentration seen by the micronuclei" is the (spatially) mean concentration in the cell. The micronuclear concentration can then be computed by regarding the micronucleus as an open, spherical system submerged in a concentration field which has, everywhere, the value of the mean concentration in the cell. The previous equations were also refined by iterating on the quasi-steady-state solutions. The equations are, then,

$$\frac{m(t)}{R} = \frac{\lambda_m}{\beta_m}\,\bar{S}(t) + \frac{1}{\beta_m}\left(1 - e^{-\beta_m t}\right), \qquad t \leqq \tau,$$

$$\frac{m(t)}{R} = \left[\frac{1}{\beta_m} + \frac{\lambda_m}{\beta_m\beta_2}\left(1 - e^{-\beta_2\tau}\right)\right] e^{-\beta_m t} + \left[\frac{\lambda_m\lambda}{\beta_m\beta_2\alpha}\left(1 - e^{-\alpha\tau}\right)\right] e^{-\alpha t}, \qquad t \geqq \tau,$$

where

$$\bar{S}(t) = \frac{\lambda}{\alpha\beta_2}\left(1 - e^{-\alpha t}\right) + \frac{1}{\beta_2}\left(1 - e^{-\beta_2 t}\right)$$

and λ, λ_m, β_m, and β_2 have fixed values; $\alpha \cdot 10^3$ has the values 4.81, 3.45, 1.36; τ has the values 15, 120, 600. For these nine cases, $m(t)/R$ was computed for $0 \leqq t \leqq 1500$

[11] J. Z. Hearon, *Bull. Math. Biophys.* **15**, 23 (1953).

[12] *Op. cit.*, p 111.

at sufficient t values to give nine smooth curves. Values of the integral

$$\int_0^t \frac{m(t)\,dt}{R} = E(\tau) - \frac{\lambda\lambda_m}{\alpha^2\beta_2\beta_m}\left(1 - e^{-\alpha\tau}\right)e^{-\alpha t}\ , \qquad t \geqq \tau\ ,$$

where

$$E(\tau) = \frac{\tau}{\beta_m}\left(1 + \frac{\lambda_m}{\beta_2} + \frac{\lambda_m\lambda}{\beta_2\alpha}\right) + \frac{1}{\beta_m^2}\left(1 + \frac{\lambda_m}{\beta_2}\right)\ ,$$

were also computed. These computations have been included in two unpublished manuscripts.[13] The general significance of these calculations has been discussed by Kimball.[14]

TWO-REGION, STEADY-STATE DIFFUSION PROBLEM

Origin: J. Z. Hearon, Mathematics Panel; R. F. Kimball, Biology Division

Participating Members of Panel: J. Z. Hearon, M. E. Fulmer

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Background and Status. In certain calculations in connection with the so-called "oxygen effect" in radiation damage and the role of H_2O_2 in x-ray mutagenesis, it is necessary to take into account the simultaneous diffusion and enzymatic consumption of H_2O_2 within biological cells. When the cells have been assayed for catalase, the enzyme which destroys H_2O_2, the rate constant for H_2O_2 consumption can be computed at once, on the assumption that the enzyme is uniformly distributed. This assumption was routinely made in such calculations (cf. "Computation of H_2O_2 in Micronucleus of *Paramecium*" and corresponding references, this report). In order to assess this assumption, the following calculations were made. For a spherical, steady-state cell the concentration, $S(r)$, satisfies the following equations:

$$D\nabla^2 S(r) - kS(r) = 0\ , \tag{1}$$

$$D\frac{\partial S}{\partial r} = h[C_0 - S(r_0)]\ , \qquad \text{at } r = r_0\ , \tag{2}$$

where k, D, and h are the rate constant, diffusion coefficient, and permeability, respectively, and r_0 is the cell radius. If k has the same value for every r, the solution of Eqs. 1 and 2 is well known to be

$$\frac{S(r)}{C_0} = A\,\frac{\sinh\,\alpha r}{r}\ , \tag{3}$$

[13] J. Z. Hearon and R. F. Kimball, "Tests for a Role of H_2O_2 in X-Ray Mutagenesis. Part I: Estimations of the Concentration of H_2O_2 Inside the Nucleus"; R. F. Kimball, N. Gaither, and J. Z. Hearon, "Tests for a Role of H_2O_2 in X-Ray Mutagenesis. Part II: Attempts to Induce Mutations by Peroxide."

[14] R. F. Kimball, *Proc. N. Y. Acad. Sci.* (in press).

where

$$A = \frac{br_0^2}{br_0 \sinh \alpha r_0 + D(\alpha r_0 \cosh \alpha r_0 - \sinh \alpha r_0)} ,$$

$$\alpha^2 = \frac{k}{D} .$$

If $k = k'$ for $0 \leqq r \leqq r_1$, and $k = 0$ for $r_1 < r \leqq r_0$, then $k' = k/\theta$, where $\theta = (r_1/r_0)^3$. If $S(r)$ and $\partial S/\partial r$ are continuous at $r = r_1$, then the solution of Eqs. 1 and 2 becomes

$$S(r) = B \frac{\sinh \beta r}{r} , \qquad 0 \leqq r \leqq r_1 ,$$

(4)

$$S(r) = a + \frac{b}{r} , \qquad r_1 < r \leqq r_0 ,$$

where

$$B = \frac{br_0^2}{br_0 \sinh \beta r_1 + D(\beta r_1 \cosh \beta r_1 - \sinh \beta r_1) + b\beta r_0(r_0 - r_1) \cosh \beta r_1} ,$$

$$a = (\beta \cosh \beta r_1)B ,$$

$$b = -(\beta r_1 \cosh \beta r_1 - \sinh \beta r_1)B ,$$

$$\beta = \frac{\alpha}{\sqrt{\theta}} .$$

Similarly, if $k = 0$ for $0 \leqq r \leqq r_1$, and $k = k''$ for $r_1 < r \leqq r_0$, then $k'' = k/\theta'$, where $\theta' = (r_0^3 - r_1^3)/r_0^3$, and

$$S(r) = \frac{\beta' br_0^2}{\Delta} , \qquad 0 \leqq r \leqq r_1 ,$$

(5)

$$S(r) = \frac{br_0^2}{\Delta} \left[\frac{\sinh \beta'(r - r_1)}{r} + \beta' r_1 \frac{\cosh \beta(r - r_1)}{r} \right] , \qquad r_1 < r \leqq r_0 ,$$

where

$$\Delta = br_0 \sinh \lambda + D(\lambda \cosh \lambda - \sinh \lambda) + \beta' r_1 br_0 \cosh \lambda + D\beta' r_0 \beta' r_1 \sinh \lambda ,$$

in which

$$\lambda = \beta'(r_0 - r_1) ,$$

$$\beta' = \frac{\alpha}{\sqrt{\theta'}} .$$

Cases 3, 4, and 5 correspond, respectively, to a uniform distribution of enzyme (the amount of which fixes k), the localization of the *same* amount of enzyme in the region $0 \leqq r \leqq r_1$, and the localization in the region $r_1 \leqq r \leqq r_0$. The ratio of the volume of the enzyme-containing region to the cell volume is θ for case 4 and is θ' for case 5. Values of $S(r)$ were computed for $10r$ values in cases 3 and 4 and for $10r$ values between r_1 and r_0 in case 5. The ratios θ and θ' were given the values 1/2, 1/10, and 1/100. The values were compared among the three cases, and, in particular, comparisons were made of the mean values

$$\bar{S} = 3 \int_0^{r_0} \frac{S(r)\, r^2\, dr}{r_0^3} .$$

Comparisons were also made between cases 3 and 5 for $\theta' = 1/10$ and for three different values of k/D.

A NUMERICAL INTEGRATION

Origin: C. W. Sheppard, Biology Division

Participating Members of Panel: G. J. Atta, A. W. Kimball, M. F. Todd

Status. A numerical quadrature was coded for the Oracle by using Simpson's Rule. The integral was of the form

$$I(E_2) = \int_0^{22} \frac{P(E_1,E_2)\, \sigma(E_1)\, R_i(E_1,E_2)}{\frac{dE}{dx}(E_1)}\, dE_1 ,$$

where $P(E_1,E_2)$ and $R_i(E_1,E_2)$ are functions involving exponentials and square roots; tables of $\sigma(E_1)$ and $\frac{dE}{dx}(E_1)$ were given.

A total of 96 cases was completed on the Oracle.

SELECTIVITY OF ION-EXCHANGE RESINS

Origin: G. H. Meyers, Chemistry Division

Participating Members of Panel: J. Z. Hearon, G. J. Atta, M. E. Fulmer, C. L. Gerberich

Background and Status. According to thermodynamic theory, the selectivity, D_{21}, of a resin for ion 2 over ion 1 is given by

$$\ln D_{21} - \frac{P\Delta V}{\beta} = \int_0^x y\, dx , \tag{1}$$

where P is the swelling pressure, ΔV is the difference in the partial molal volumes of the ions, $x = -\ln a_w$, where a_w is the water activity in the resin, and

$$y = \left(\frac{\partial 1/m}{\partial x_2}\right)_{X_2} , \tag{2}$$

where $m = m_1 + m_2$ is the total molality of the ions in the resin, and X_2 is the mole

fraction of ion 2. The quantity $y(x)$ is obtained from the slope of $1/m$ as a function of X_2 evaluated at a given value of X_2 and various values of ln a_w. In general, for each of five fixed values of X_2, the value of $y(x)$ was available for nine values of x. It was desired to fit these five curves $y(x)$, compute the integrals in Eq. 1, and compare the D_{21}, so computed, with the independently and directly determined values of D_{21}. It was found that the data could be fitted by

$$y(x) = \frac{a}{b + x} .$$

Least-squares fit for the linear function

$$\frac{1}{y} = \frac{b}{a} + \frac{1}{a}\left(\frac{1}{x}\right)$$

was obtained, standard errors for a and b were computed for five curves, and the results were returned to the originator. It is planned to obtain Eq. 2 by numerical differentiation and to fit the remaining data to the function $y(x) = P^{-1}(x)$, where P is a polynomial of degree $\leqq 10$. This problem is presently being coded for the Oracle, since there are some 15 ion-resin systems (with five curves each) to be analyzed.

PATH-LENGTH DISTRIBUTION

Origin: G. H. Jenks, Chemistry Division

Participating Members of Panel: J. Z. Hearon, A. C. Downing

Background and Status. Given a containing wall and a solution in which fission products arise, it is required to know the number, $N(h)\,dh$, of particles whose paths terminate at the depth h within dh, in the wall, where h is reckoned normal to the solution-wall interface. Taking the empirical fact that for many types of particles the probability of traveling the distance λ or greater is exp $(-\lambda/R)$, where R is characteristic of the particle and the medium, it follows that the probability of the particle stopping in the interval $d\lambda$ after traveling the distance λ is $(1/R)$ exp $(-\lambda/R)$. It can then be shown that

$$N(h) = \int_0^\infty N_0\, dx \int_{-\pi}^{\pi} P(x,\theta,h)\,\frac{d\theta}{2\pi} , \tag{1}$$

where N_0 is the number of particles which arise per unit volume of solution, and $P(x,\theta,h)$ is the probability that a particle originating at (perpendicular) distance x from the wall with angle θ between the path and the normal to the wall penetrates the (perpendicular) distance h into the wall. With

$$P(x,\theta,h) = \frac{1}{R_w \cos\theta} \exp\left[\frac{1}{-R_w \cos\theta}\left(x\,\frac{R_w}{R_s} + h\right)\right] ,$$

where R_s and R_w are the R values for solution and wall, Eq. 1 becomes

$$N(h) = \frac{N_0}{\pi} \cdot \frac{R_s}{R_w} \int_0^{\pi/2} \exp\left(\frac{-h}{R_w \cos\theta}\right) d\theta \quad . \tag{2}$$

Numerical values of the integral are available as a function of $k = h/R_w$. A table of values covering $0 \leqq k \leqq 3.6$ was prepared and returned to the originator.

OSMOTIC COEFFICIENTS FOR ION-EXCHANGE RESINS

Origin: G. H. Meyers, Chemistry Division

Participating Members of Panel: J. Z. Hearon, G. J. Atta

Background and Status. The osmotic coefficient ϕ is defined by

$$\phi = \frac{k \ln a_w}{m} \quad , \tag{1}$$

where k is a known constant, a_w is the activity of water in the resin, and m is the molality of counter-ions in the resin. The coefficient ϕ is determined by equilibrating the resin with known vapor pressures of water, measuring the weight of water taken up by the resin, and computing m from the known capacity of the resin. It was desired to study the function

$$\phi = \phi_0 + \frac{am}{1 + bm} \tag{2}$$

and, in particular, to study the parameters a and b as a function of ionic radius, etc. Data are available for some 20 systems and are currently being collected for others. Equation 2 was fitted by the following device: Let $Q(x)$ be $1/(\phi - \phi_0)$, where x is $1/m$. Then

$$Q(x) = \frac{b}{a} + \frac{x}{a} \quad . \tag{3}$$

For arbitrary values of ϕ_0 the least-squares fit of Eq. 3 is obtained. For each ϕ_0, and the corresponding values of a and b, the quantity $V = \Sigma[Q(x) - \hat{Q}(x)]^2$ is computed, where $\hat{Q}$ is the expected value of Q from Eq. 3. From a plot of V against ϕ_0, the minimum value of V is located, and the values of ϕ_0, a, and b at minimum V are the least-square values of the parameters. This procedure was completed for seven systems, and the results were returned to the originator.

DAMAGE TO TISSUE FROM NEUTRON BEAMS

Origin: W. S. Snyder, Health Physics Division

Participating Members of Panel: N. M. Dismuke, M. E. Fulmer, C. D. Zerby

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Status. Maximum permissible flux determinations have been completed for neutron beams of 0.1, 0.02, 0.005, and 0.0001 Mev.

The model was an infinite 30-cm slab of tissue irradiated by monoenergetic neutrons normally incident on one face of the slab. Interaction types considered were elastic scatterings in H, O, C, and N and the reactions H(n,γ) and N(n,p). Cross sections were obtained from an AECU report.[15]

In this computation, energy losses due to the various interaction types were estimated statistically by use of the Monte Carlo method. To obtain the flux determinations, the energy losses were weighted with RBE factors which were assumed to be constants for each of the interaction types.

For each beam, 10,000 neutron histories were computed in groups of 1000 neutrons. For each group, the resulting gamma source was normalized to give at least 1000 gamma rays per group for the gamma-ray Monte Carlo problem. All computations were carried out on the Oracle.

The following tabulations as functions of slab penetration were made for each beam:

1. proton interaction,
2. heavy-particle interaction,
3. gamma-ray interaction,
4. the total energy transmitted to the slab,
5. the damage to the slab [i.e., the sum of (1), (2), and (3) weighted with RBE factors]; energy was transmitted to the tissue slab by means of the reactions indicated in (1), (2), and (3).

Since the problem described above was programmed, the National Committee on Radiation Protection has issued a handbook[16] which recommends a different procedure of weighting the relative biological effectiveness. The possibility of modifying existing codes to follow this standardized treatment is being investigated. At the same time changes are being considered which will allow beam energies to be as high as 10 Mev.

BOND STRENGTHS OF ORGANIC MOLECULES

Orgin: J. G. Burr, Chemistry Division

Participating Member of Panel: A. C. Downing

Background and Status. Problems have arisen in the Chemistry Division regarding the bond strengths of certain organic molecules and regarding the total π-electron energy of certain intermediates hypothesized to occur in organic reactions. Solutions to these problems have been attempted by using the semiempirical theory in which molecular orbitals are approximated by linear combinations of atomic orbitals (the LCAO approximation). This approximation ultimately requires the determination of the principal values and principal directions of the system of equations corresponding to

[15] D. H. Hughes *et al.*, *Neutron Cross Section. A Compilation of the AEC Neutron Cross Section Advisory Group*, AECU-2040 (May 15, 1952).

[16] *Permissible Dose from External Sources of Ionizing Radiation*, National Bureau of Standards Handbook 59 (Sept. 24, 1954).

the secular determinant

$$\det |H_{\mu\nu} - ES_{\mu\nu}| = 0 \ .$$

Here, $H_{\mu\nu}$ is a symmetric matrix derived from the Hamiltonian operator, E is the energy of the possible molecular orbitals, and the elements of the matrix $S_{\mu\nu}$ are the integrals describing the overlap of the μth and νth atomic orbitals. The size and complexity of the secular determinant depend upon the size and complexity of the organic molecule.

For numerical reasons, it is almost universally assumed that the individual atomic orbitals are orthogonal, thus making $S_{\mu\nu}$ the identity matrix. Even with this assumption, a thorough consideration of such problems by the LCAO approximation is beyond the profitable limits of manual calculation. However, with the aid of the standard Oracle subroutines for calculating the principal directions of symmetric matrices, a large number of these secular systems have been studied.

Considerable improvement in the accuracy of the LCAO approximation is possible if the orthogonality of the atomic orbitals is not assumed. In fact, calculations indicate that the overlap integral $S_{\mu\nu}$ for adjacent carbon π-electrons is in the vicinity of 0.25. When $S_{\mu\nu}$ is not the identity matrix, the numerical problem is no longer that of finding the characteristic vectors of a symmetric matrix, since $S^{-1}H$ is not symmetric even though S and H are symmetric. Methods for handling such problems with the aid of the Oracle are now being studied by the Mathematics Panel.

TABULATION OF DISTRIBUTION OF CENTER-OF-MASS ENERGIES AS A FUNCTION OF CENTER-OF-MASS ANGLES FOR TWO CROSSED MOLECULAR BEAMS

Origin: S. Datz, Chemistry Division

Participating Member of Panel: E. C. Long

Background and Status. Values for the tabulation of the distribution of center-of-mass energies were obtained for the equations

$$P(\theta,E,T_1,T_2,m_1,m_2) = \frac{1}{2}\left[\frac{\left(\frac{m_1}{m_2}\right)^2 (m_1 + m_2)^2}{m_1 m_2 k^2 T_1 T_2}\right]^2 \frac{\tan^3\theta \sec^2\theta}{\left[\left(\frac{m_1}{m_2}\right)^2 + \tan^2\theta\right]^4} E^3 \epsilon^F \ ,$$

$$F = -E\,\frac{m_1 + m_2}{k T_1 m_2}\left[\frac{\frac{m_1 T_1}{m_2 T_2} + \tan^2\theta}{\left(\frac{m_1}{m_2}\right)^2 + \tan^2\theta}\right] .$$

Tabulation was made of $P(E,\theta) = f(\theta)$, E fixed. Ranges of θ and E were:

$$2.5^\circ \leqq \theta \leqq 97.5^\circ , \qquad \Delta\theta = 2.5^\circ,$$

$$0 < E \leqq 10{,}000 , \qquad \Delta E = 200 \text{ cal.}$$

Complete calculations were obtained for two values of T_2.

Subroutines used in this problem were: two-line floating-point input and output conversions; two-line floating-point arithmetic; sin θ, cos θ; and floating-point exponential. The problem has been completed.

SUMMATION OF A DOUBLE FOURIER SERIES

Origin: H. A. Levy, Chemistry Division

Participating Member of Panel: V. C. Klema

Background and Status. The problem consists in computing the following double Fourier series:

$$F(x,y) = \sum_{h=0}^{H} \sum_{k=-K}^{K} (2 - \delta_0 h) [A_{hk} \cos 2\pi(hx + ky) + B_{hk} \sin 2\pi(hx + ky)]$$

for x,y at intervals Δx, Δy on the rectangle $(x_1,y_2) - (x_2,y_1)$, for $x_1 < x_2$ and $y_1 < y_2$.

The coefficient $(2 - \delta_0 h)$ requires δ_{mn} to be zero if $m \neq n$, and δ_{mn} to be unity if $m = n$. Thus $(2 - \delta_0 h)$ is 1 for $h = 0$, 2 for $h > 0$. This coefficient arises from a symmetry relation on the A's and B's which allows the above sum to be substituted for a sum in which h originally ran from $-H$ to H.

Given x_1, x_2, y_1, y_2, Δx, Δy, H, K, and the data A_{hk}, B_{hk}, the Oracle program computes sines and cosines as needed and sums the series to punch the value of the function. Current time estimates show a total computing time of 3 sec for $F(x,y)$ for each x and y for $H = 11$, $K = 10$; IBM results were used to check the computation.

SCATTERING BY A CYLINDRICAL SHELL WHICH SURROUNDS AN ABSORBING MEDIUM

Origin: H. A. Levy, Chemistry Division

Participating Members of Panel: S. G. Campbell, M. F. Todd

Background and Status. In order to relate the scattering by the filled shell, which surrounds an absorbing medium, with the scattering by the empty shell, it was necessary to evaluate the integral

$$A(B,\phi) = \frac{1}{2\pi} \left\{ \int_\phi^\pi e^{-B\sin\alpha}\, d\alpha + \int_0^\phi e^{-B[\sin\alpha + \sin(\phi-\alpha)]}\, d\alpha + \phi \right\}$$

for $B = 0, 0.1, 0.2, \ldots, 5.0$; $\phi = 0, 10^\circ, 20^\circ, \ldots, 180^\circ$.

This integral was coded for the Oracle by using 128-point Gaussian integration. The problem has been completed, and the results were given to the originator.

TRACER KINETICS

Origin: G. A. Ropp, Chemistry Division

Participating Member of Panel: J. Z. Hearon

Background and Status. It is usually asserted that a radioactive exchange reaction obeys first-order kinetics regardless of the number of exchangeable groups involved. The various proofs presented are not entirely satisfactory from the standpoint of detailed chemical kinetics. It was desired to have a satisfactory formulation for the exchange between C^{14}-tagged acetone and aluminum isopropoxide and to state how the parameters of the time-specific activity curve are influenced by the presence of a side equilibrium, namely, the subsequent exchange between tagged isopropoxide and isopropyl alcohol. Consider the reactions

$$K^* + A_{i-1} \rightleftharpoons A_i + K \quad , \qquad i = 1, 2, 3 \ ,$$

where K^* and K are tagged and untagged acetone, respectively, and A_k, $k = 0, 1, 2, 3$, is aluminum isopropoxide in which k isopropyl groups are tagged. If k_i and k_{-i} are the forward and reverse rate constants for the ith reaction, the rate equation for K^* is

$$\frac{dK^*}{dt} = -K^* \sum_{j=1}^{3} k_j A_{j-1} + K \sum_{j=1}^{3} k_{-j} A_j \ .$$

If

$$R = k(K + K^*) \sum_{j=0}^{3} A_j$$

is the total exchange rate, where k is the intrinsic rate constant for the reaction, then

$$\frac{dK^*}{dt} = R(S_A - S_K) \ ,$$

where $S_A = \sum_{j=0}^{3} jA_j/3 \sum_{j=0}^{3} A_j$ and $S_K = K^*/(K + K^*)$ are the specific activity of tagged groups in A and the specific activity of the acetone, provided

$$k_j = \frac{(3 - j + 1)k}{3} \ , \qquad k_{-j} = \frac{jk}{3} \ , \qquad j = 1, 2, 3 \ ,$$

that is, provided the $k_{\pm j}$ are equal to k except for the statistical factors. If K^*_{eq} is the equilibrium value of K^*, and the initial conditions are $A_j = 0$, $j = 1, 2, 3$, at $t = 0$, then

$$K^*_{eq} - K^*(t) = K^*_{eq} e^{-\beta t} \ , \tag{1}$$

where $\beta = R/\sum_{j=0}^{3} A_j + R/(K + K^*)$ is the effective first-order rate constant. If the reactions

$$A_i + B \rightleftharpoons B^* + A_{i-1} \quad , \qquad i = 1, 2, 3 \ ,$$

are also occurring, where B^* and B are tagged and untagged isopropyl alcohol, then, by the same arguments,

$$\frac{dB^*}{dt} = R_2(S_A - S_B) \quad ,$$

where

$$R_2 = k'(B + B^*) \sum_{j=0}^{3} A_j \quad ,$$

$$S_B = \frac{B^*}{B + B^*} \quad .$$

If the alcohol exchange is essentially at equilibrium, then

$$B^* \cong \frac{B_t A^*}{A} \quad ,$$

where $B_t = B^* + B$. If, initially, all the tag is in K, so that the initial value of K_0^* is

$$K_0^* = A^* + K^* + B^* \quad ,$$

then Eq. 1 holds if β is now defined by

$$\beta = \frac{R}{\sum_{j=0}^{3} A_j} + \frac{R}{B_t} + \frac{R}{A^* + A} \quad .$$

SCATTERING CALCULATION FOR INTERSECTING BEAMS OF K AND HBr

Origin: S. Datz, Chemistry Division

Participating Members of Panel: S. G. Campbell, M. F. Todd

Background and Status. In order to calculate the activation energy of the reaction between K and HBr, it was necessary to evaluate the function

$$G = -\frac{\alpha_1^2 \alpha_2^2}{(\alpha_1 - \alpha_2)^2} \left\{ \frac{e^{-\alpha_2 v_{12}^2}}{\alpha_2} \left[\frac{3\alpha_2 - \alpha_1}{\alpha_2(\alpha_1 - \alpha_2)} - v_{12}^2 \right] - \frac{e^{-\alpha_1 v_{12}^2}}{\alpha_1} \left[\frac{3\alpha_1 - \alpha_2}{\alpha_1(\alpha_1 - \alpha_2)} + v_{12}^2 \right] \right\} ,$$

where

$$\alpha_1 = 20.36789 \cdot \frac{1}{T_1} \quad ,$$

$$\alpha_2 = 9.84163 \cdot \frac{1}{T_2} \quad ,$$

$$v_{12}^2 = \frac{E}{13.181} ,$$

$$100 \leqq T_1 \leqq 800 , \quad \Delta T_1 = 20^\circ ,$$
$$500 \leqq T_2 \leqq 1000 , \quad \Delta T_2 = 20^\circ ,$$
$$500 \leqq E \leqq 10{,}000 , \quad \Delta E = 500 .$$

The function was coded for the Oracle. The problem has been completed, and the results were given to the originator.

A TRIPLE INTEGRATION PROBLEM[17]

Origin: H. Zeldes, Chemistry Division

Participating Members of Panel: S. G. Campbell, M. F. Todd

Background and Status. In the study of an environmental effect on atomic hydrogen hyperfine structure in acids, it was necessary to evaluate certain triple integrals of the form

$$\int_{r=0}^{\infty} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \frac{\cos\theta \sin^2\theta}{r} e^{-2|r_1|/a_0} \, dr \, d\phi \, d\theta$$

and

$$\int_{r=0}^{\infty} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \frac{1 - 3\cos^2\phi}{r} e^{-2|r_1|/a_0} \, dr \, d\phi \, d\theta ,$$

where $r_1^2 = R^2 + r^2 - 2rR (\sin\theta_1 \sin\theta \cos\phi + \cos\theta_1 \cos\theta)$.

The numerical integration was performed on the Oracle by using a standard Gaussian integration subroutine. The code has been run for six values of R, and the results were given to the originator.

MECHANICS OF THE THREE-BODY BREAKUP OF Li^6 INTO ALPHA, PROTON, AND NEUTRON PARTICLES

Origin: C. D. Moak, Physics Division

Participating Member of Panel: E. C. Long

Background and Status. In the study of the mechanics of the three-body breakup of Li^6, values were obtained for roots of the quadratic equation

$$\sqrt{E_n} = (0.2012 \sqrt{E_p} \cos\theta - 0.1907 \sin\theta)$$
$$\pm \sqrt{(0.2012 \sqrt{E_p} \cos\theta - 0.1907 \sin\theta)^2 + 9.836 - 1.0007 E_p} ,$$

where E_n and E_p are energies of neutron and proton, respectively, and θ is the angle of emergence. The quantity E_p was varied for fixed values of θ, the ranges of θ and E_p being

$$-90^\circ \leqq \theta \leqq 90^\circ ,$$
$$0 \leqq E_p \sim 10 .$$

[17] H. Zeldes and R. Livingston, *Phys. Rev.* **96**, 1702 (1954).

The upper limit of E_p was that value which caused the radical to become imaginary.

Subroutines used in this problem were: two-line floating-point input and output conversions; two-line floating-point arithmetic; sin θ, cos θ; and $\sqrt{n}$. This problem has been completed.

INTERNAL CONVERSION COEFFICIENTS OF THE M SHELL

Origin: M. E. Rose and A. Glassgold, Physics Division

Participating Members of Panel: S. E. Atta, W. C. Sangren

Background. It is desired that a large number of internal conversion coefficients be computed for the five subshells of the M shell, for variable gamma-ray energies, for variable atomic numbers, and for both electric and magnetic multipoles. The problem uses many formulas and equations, as well as complex arithmetic. The problem will employ the use of the following subroutines: hypergeometric series for complex parameters and complex argument, sin $(x + iy)$, $\Gamma(x + iy)$, $(V + iW)^{x+iy}$, ln $(x + iy)$, $\tan^{-1} y/x$, $e^{(x+iy)}$, sin x, and cos x.

Status. Many of the subroutines have been checked out, while the remaining ones are near completion. A general flow diagram and other plans have been prepared for the problem as a whole.

A COULOMB WAVE FUNCTION PROBLEM

Origin: L. C. Biedenharn, Research Participant, Physics Division

Participating Members of Panel: S. E. Atta, W. C. Sangren

Background. It was desired that the following equation be evaluated:

$$I = (-1)^{L'+1}(1 - \rho)^{-2L'-2}\,\Gamma(2L' + 2)\left(\frac{\rho + 1}{\rho - 1}\right)^{-1-L'-i\rho\eta}$$

$$\cdot \sum_m \frac{(L' + 3 - i\eta)_m\,(2L' + 2)_m}{(2L' + 6)_m\, m!}\; {}_2F_1\left(L' + 1 - i\rho\eta, -m;\ 2L' + 2;\ \frac{2}{1 - \rho}\right)\left(\frac{2\rho}{1 + \rho}\right)^m ,$$

where

$$L' = 0, 1, 2, \ldots ,$$
$$0 < \rho < 1 ,$$
$$1 < \eta < 100 .$$

The computation of $\sum_m$ is complicated by the fact that although there are a finite number of terms, ${}_2F_1[L' + 1 - i\rho\eta, -m;\ 2L' + 2;\ 2/(1 - \rho)]$ causes each term to be quite large $\left[\sim\left(\frac{2}{1 - \rho}\right)^m\right]$, and the sum is quite small. The region of most physical interest is $\rho \sim 9/10$. Three different methods were programmed as an attempt to avoid this complication. All three failed to accomplish the desired results.

Since the function at $\rho \sim 1$ has discontinuous properties which are particularly pronounced for $\eta_1 \neq \eta_2$, the following integral was evaluated as a test for a new method of attack:

$$I = \int_0^\infty r^{-3} F_0(r;\eta = 1) F_2(r;\eta = 3/2)\, dr \quad .$$

Status. It is believed that a new workable method has been found for the problem and that this method will be programmed sometime in the future.

EVALUATION OF OVERLAPPING POWER SERIES

Origin: J. E. Faulkner, Physics Division

Participating Member of Panel: M. D. George

Status. Given the function

$$\phi(x) = \frac{1}{2} + \frac{2}{\pi^2}\left[F(r) + \ln(1 - r)\ln\frac{r}{2}\right] \quad ,$$

where, for small x,

$$F(r) = \sum_{j=1}^{\infty} a_j r^j \ , \quad a_j = j^{-2} - j^{-1}\sum_{k=1}^{j-1} k^{-1}\, 2^{-k} \ ,$$

$$a_1 = 1 \ , \quad r = 1 - \sqrt{x^2 + 1} + x \quad ,$$

and, for large x,

$$\phi(x) = 1 - \frac{4}{\pi^2}\sum_{j=0}^{\infty} \frac{\tau^{2j+1}}{(2j + 1)^2} \quad ,$$

a graph of $\phi(x)$ was desired such that it could be read to within an accuracy of 5% or better. The expansion about the origin was carried out to the point where 25 terms were required for six-digit convergence; the expansion about infinity was then used, and agreement of the two expansions in the overlapping region was checked to six decimal digits. The function was then graphed, and the graphs were turned over to the originator.

LEAST-SQUARES FITTING OF ANGULAR DISTRIBUTION DATA

Origin: J. L. Fowler, Physics Division

Participating Member of Panel: V. C. Klema

Background and Status. It is desired to fit angular distribution data to a polynomial in cos θ and to a polynomial in $P_n(x)$, the Legendre polynomial.

The Oracle program accepts data taken at a maximum of 32 angles, calculates weighting factors from the standard deviations, σ_i, produces, if desired, the $P_n(x)$ from the recurrence relation $(n + 1) P_{n+1}(x) - (2n + 1) xP_n(x) + nP_{n-1}(x) = 0$, and forms the system of normal equations.

Along with the solution of the system of equations is produced the quantity

$$s^2 = \frac{1}{n - (k + 1)}\left[\Sigma w_i(y_i - y_i \text{ cal})\right] \ ,$$

where n is the number of points, k is the degree of the polynomial to which the data are fit, w_i are the weighting factors, y_i represents the data, and y_i cal are the predicted values from the fit. .

The program carries out necessary scaling internally and will fit data to a polynomial of even degree or to a polynomial including terms of odd degree.

MIXED-MIXED GAMMA-GAMMA ANGULAR CORRELATION FUNCTIONS

Origin: E. D. Klema and F. K. McGowan, Physics Division

Participating Member of Panel: V. C. Klema

Background and Status. The previous code for angular correlation functions is for the case where one gamma ray is pure and the other is a mixture of electric and magnetic radiation. The current Oracle program is an extension to the case in which both gamma rays are mixed radiation.

SCATTERING CALCULATIONS FOR BEVELED CRYSTALS

Origin: P. R. Bell, Physics Division

Participating Members of Panel: S. G. Campbell, C. L. Gerberich

Background and Status. Given a cylindrical crystal of radius r and length t with its forward face beveled by an angle of θ radians (so that r_1 is the radius of the beveled face), the efficiency of the crystal is calculated by evaluating the integral

$$T_b(\tau) = \frac{1}{2}\int_0^{\alpha_i} \sin\alpha[1 - e^{-\tau x(\alpha)}]\, d\alpha \quad .$$

The function $x(\alpha)$ has three separate forms, depending upon the distance b of the source from the center of the forward face of the crystal along the axis of the crystal. If

$$b_0 = 0 \ , \qquad \alpha_1 = \tan^{-1}\frac{r}{b+t} \ ,$$

$$b_1 = r_1 \tan\theta \ , \qquad \alpha_2 = \tan^{-1}\frac{r}{b}$$

$$b_2 = \frac{r_1 t}{r - r_1} \ , \qquad \alpha_3 = \tan^{-1}\frac{r_1}{b} \ ,$$

$$\alpha_4 = \tan^{-1}\frac{r}{b + (r - r_1)\tan\theta} \ ,$$

then in the range $b_0 \leqq b \leqq b_1$, $\alpha_i = \alpha_3$ and

$$x = t\sec\alpha \qquad \text{for } 0 \leqq \alpha \leqq \alpha_1 \ ,$$

$$x = \sin\theta\sec(\theta + \alpha)(b\tan\alpha - r_1) \qquad \text{for } \alpha_4 \leqq \alpha \leqq \alpha_3 \ ,$$

$$x = r\csc\alpha - b\sec\alpha \qquad \text{for } \alpha_1 \leqq \alpha \leqq \alpha_4 \ .$$

For $b_1 \leqq b \leqq b_2$, $\alpha_i = \alpha_4$ and

$$x = t \sec \alpha \qquad \text{for } 0 \leqq \alpha \leqq \alpha_1 ,$$

$$x = r \csc \alpha - b \sec \alpha \qquad \text{for } \alpha_1 \leqq \alpha \leqq \alpha_3 ,$$

$$x = \frac{\cos \theta[r \cot \alpha - b - (r - r_1) \tan \theta]}{\cos (\theta + \alpha)} \qquad \text{for } \alpha_3 \leqq \alpha \leqq \alpha_4 .$$

For $b > b_2$, $\alpha_i = \alpha_4$ and

$$x = t \sec \alpha \qquad \text{for } 0 \leqq \alpha \leqq \alpha_3 ,$$

$$x = \frac{\sin \theta(b \tan \alpha - r_1)}{\cos (\theta + \alpha)} \qquad \text{for } \alpha_3 \leqq \alpha \leqq \alpha_1 ,$$

$$x = r \csc \alpha - b \sec \alpha \qquad \text{for } \alpha_1 \leqq \alpha \leqq \alpha_4 .$$

If the crystal is not beveled, then for all b, $\alpha_i = \alpha_2$ and

$$x = t \sec \alpha \qquad \text{for } 0 \leqq \alpha \leqq \alpha_1 ,$$

$$x = r \csc \alpha - b \sec \alpha \qquad \text{for } \alpha_1 \leqq \alpha \leqq \alpha_4 .$$

In the case under consideration, the basic constants are

$$r = 3.81000762 \text{ cm} ,$$

$$t = 7.62001524 \text{ cm} ,$$

$$r_1 = 2.54000508 \text{ cm} ,$$

$$\theta = \frac{\pi}{4} .$$

The Gaussian 16-point numerical quadrature formula, which was coded and tested originally for this problem by C. L. Gerberich, was used for the integration; convergence of the integration process was checked to nine decimal digits. The program calculated and punched both the absolute and the relative efficiencies for both the beveled and the nonbeveled crystals for 13 selected values of τ and, for each value of τ, for 32 different values of h.

TABULATION OF ANGULAR DISTRIBUTION OF SCATTERING FUNCTION

Origin: M. F. Valerino, Physics Division

Participating Member of Panel: S. G. Campbell

Background and Status. The integral

$$T(\theta) = \sin \theta \int_{x=0}^{\infty} \frac{\exp \left[-\left(x + \sqrt{0.0225 - 0.30x \cos \theta + x^2}\right)\right]}{0.0225 - 0.30x \cos \theta + x^2} \, dx$$

was evaluated by Gaussian numerical integration on the Oracle for $\theta = 0°$, $(1/16)°$, $(2/16)°$, ... , $(15/16)°$, $1°$, $2°$, ... , $9°$, $12°$, $15°$, ... , $180°$. Despite the great range of the integrand [the integral is singular at $\theta = 0°$, but $T(\theta)$ is not], the calculation was done in fixed-point form; however, it was necessary to make the program self-scaling.

For each value of θ, the program calculated first the maximum value of the integrand, then scaled it accordingly before entering the integration routine. It was observed that such a procedure, when applied to numerical integration problems in which the range of the integrand is very large, can be made to produce as much accuracy as floating-point operations, with essentially the speed of a fixed-point calculation.

AIR-SCATTERING CALCULATION

Origin: F. H. Murray, Physics Division

Participating Members of Panel: S. G. Campbell, M. F. Todd

Background and Status. The problem in the air-scattering calculation was to evaluate the triple integrals

$$I_1 = \frac{\sigma}{16\pi^2 D} \int_{\beta=0}^{\pi} \int_{\phi=0}^{\pi/2} e^{-1.25/\sin\beta\sin\phi}\, d\beta\, d\phi \int_{\alpha=0}^{\operatorname{arc\,cot}(D/H\cos\phi-\cot\beta)} f(\alpha)\, \phi_\sigma(\alpha+\beta)\, d\alpha$$

and

$$I_2 = \frac{\sigma}{16\pi^2 D} \int_{\beta=0}^{\pi} \int_{\phi=0}^{\pi/2} e^{-1.25/\sin\beta\sin\phi}\, d\beta\, d\phi \int_{\alpha=0}^{\pi-\beta} f(\alpha)\, \phi_\sigma(\alpha+\beta)\, d\alpha\,,$$

where

$$f(\alpha) = 1,\ \cos\alpha,\ \cos^2\alpha,\ \text{or}\ \cos^3\alpha,$$

$$\phi_\sigma(\alpha+\beta) = 1 + 0.3\,(\cos\alpha\cos\beta - \sin\alpha\sin\beta)\,.$$

The first integration was done analytically, and the resulting double integral was evaluated numerically on the Oracle by using the standard double Gaussian integration subroutine. Fourteen values of D/H were used in the calculation. Air-scattering is equal to the sum of I_1 and I_2. The results have been given to the originator.

RANDOM NUMBER TESTS

Origin: R. R. Coveyou, Research Director's Division

Participating Member of Panel: M. E. Fulmer

Background and Status. The objective of the random number tests was to investigate various methods of generating pseudo-random numbers for Monte Carlo calculations. At present, the analysis of data for this problem has been suspended in favor of more pressing work. One tentative conclusion has been reached: Of the methods tested, only the so-called "congruence" method showed adequate statistical reliability.

FISSION-PRODUCT PROBLEM

Origin: R. A. Charpie, Research Director's Division

Participating Members of Panel: S. G. Campbell, C. P. Hubbard, M. F. Todd

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Background and Status. The Oracle code for the fission-product problem, mentioned in the reference, was modified to include two additional differential equations. The computation time for this modified code was excessive for certain chains. This was partially

due to the small interval size chosen automatically by the code in these cases. Additional difficulties arose with this code in those chains where some of the nuclides were missing. To eliminate this difficulty and to reduce computation time, the system of equations has been written to evaluate these solutions for the desired values of irradiation and cooling times. The new code is now ready for production.

CALCULATION OF ENERGY-LEVEL VALUES

Origin: H. W. Morgan, Stable Isotope Research and Production Division

Participating Member of Panel: M. R. Arnette

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Background and Status. Another set of parameters for the calculation of energy-level values was received. The same code that was used for the previous seven sets was used for this set of parameters, and the resulting answers were sent to the originator.

DETERMINATION OF THE FORCE CONSTANTS OF FORMYL FLUORIDE

Origin: H. W. Morgan, Stable Isotope Research and Production Division

Participating Members of Panel: R. C. F. Bartels, A. C. Downing, E. C. Long

Status. The desired force constants of formyl fluoride were obtained; the problem has been completed. (For a description of the mathematical problem, cf. "Inverse Characteristic Value Problem," this report.)

SAFETY CALCULATIONS FOR THE HRT

Origin: P. R. Kasten, Reactor Experimental Engineering Division

Participating Member of Panel: C. P. Hubbard

Reference: Mathematics Panel Semiannual Report, ORNL-1751

Background and Status. The system of four first-order differential equations discussed in ORNL-1751 has been modified to represent the kinetic conditions of a reactor with a blanket. The new system consists of seven first-order differential equations. As before, the purpose of the calculations is to determine maximum power and maximum pressure within the core and the blanket for various values of certain parameters. The equations were solved by using the mid-ordinate method with two starting values. All calculations were performed in floating-point form because of the great range of the functions involved. The problem is now in production status.

THERMAL EFFECTS IN A CAPTURING MEDIUM

Origin: R. K. Osborn, ARE Division

Participating Member of Panel: M. E. Fulmer

Background and Status. Extensive calculations are being performed to determine the energy spectrum of neutrons slowing down in a capturing medium. Monte Carlo methods are being employed, and a survey is in progress of the dependence of the spectrum upon mass and scattering cross section of the moderator, capture cross section of the absorber, and temperature of the medium. The numerical results represent the scattering density in

512 speed intervals from 0 to 32 times thermal speed. These data are being converted to flux and number density and will be plotted vs speed.

"M" LINE CHARACTERISTICS – MATRIX SOLUTION

Origin: Tennessee Valley Authority

Participating Members of Panel: M. R. Arnette, M. E. Fulmer; M. Hochdorf, Tennessee Valley Authority

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Status. The inverse of the F matrix which caused considerable delay in the problem associated with "M" line characteristics has now been obtained. The trouble was traced to an error in the input data. The F matrix contained one element which was off by a factor of 10 and which caused the F^{-1} to lose its symmetric pattern. In checking the inverse code, two columns of $F \cdot F^{-1}$ were calculated on the Friden. It is expected that by the end of another week the $Z = Z_1 - AF^{-1}B - DG^{-1}H$ will have been completed.

MULTIGROUP REACTOR CALCULATIONS

Origin: R. A. Charpie, Research Director's Division

Participating Members of Panel: J. H. Alexander, N. D. Given

References: Mathematics Panel Semiannual Progress Reports, ORNL-1588, -1662, -1751

Background and Status. The Eyewash program, which is the latest multigroup program written for the Univac, has been in the production status since last May. Because it is a very general program, there is a great deal of flexibility in reactor description. For this reason, Eyewash has not only been used by the ARE Division and the HR Project of ORNL but has also been made available to other groups, such as KAPL, Westinghouse, NDA, Wright-Patterson, Argonne, and the Babcock and Wilcox Co. For the use of all those interested in multigroup calculations, a complete report will be issued soon.