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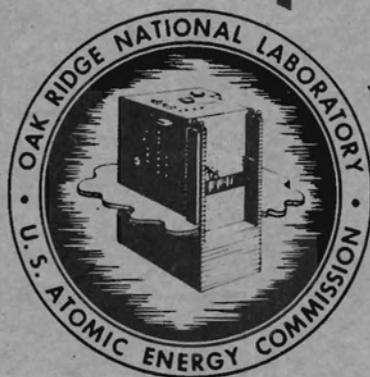
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SEMIANNUAL PROGRESS REPORT
FOR
PERIOD ENDING JUNE 30, 1955

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SEMIANNUAL PROGRESS REPORT**

for

Period Ending June 30, 1955

A. S. Householder, Chief

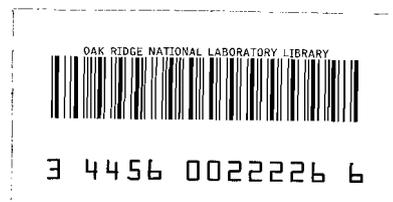
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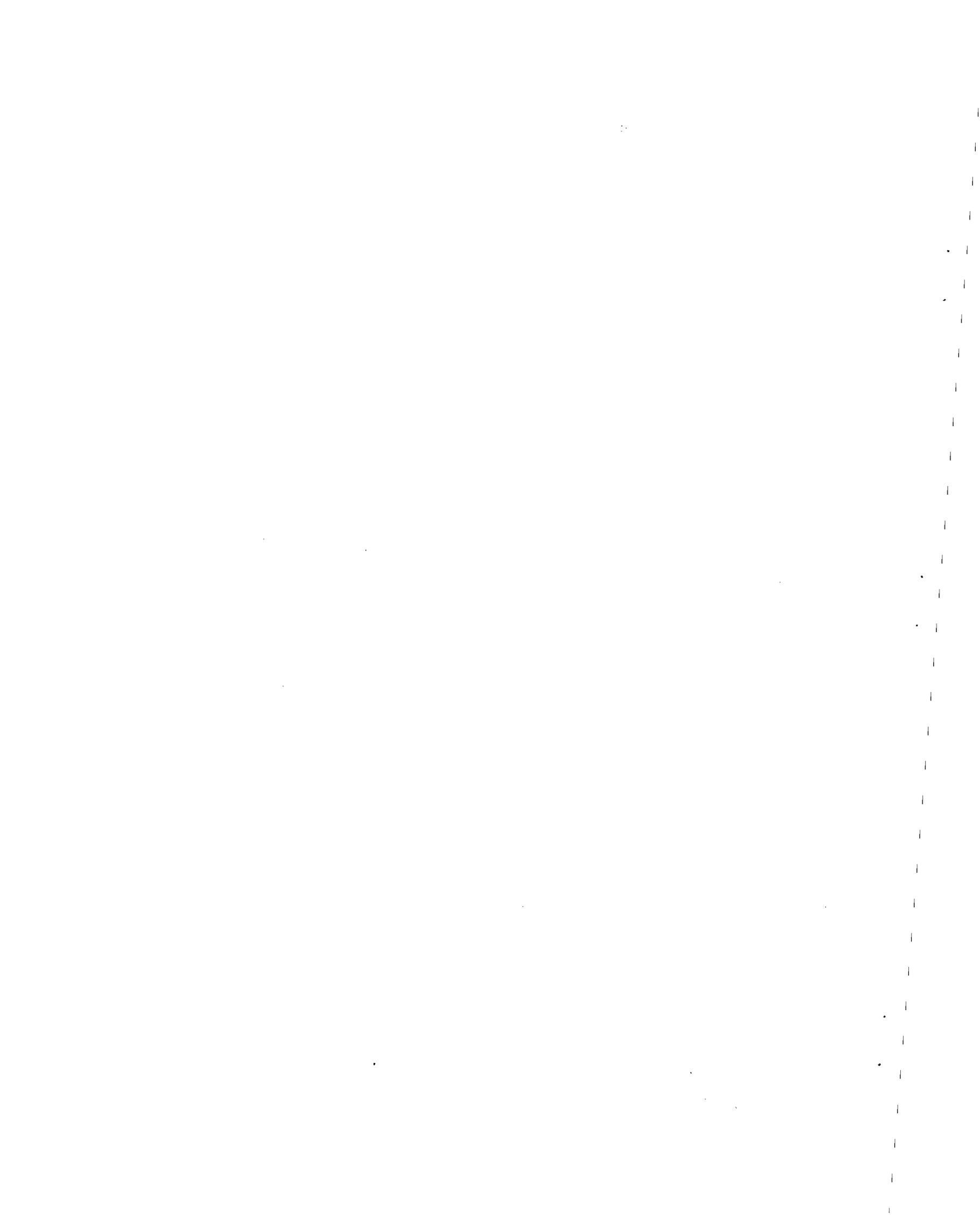
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INTRODUCTION

THE ORACLE

From January through June, a total of 1679 hr of computing time was used by programmers in "debugging" and running problems. Over a period of four months, one shift has been used daily in completing the electrical installation of the magnetic-tape memory. The other two shifts have been utilized for problem solving. Work is continuing on the new input-output system.

LECTURES

ORINS Lectures. – The following lectures were given under the Traveling Lecture Program:

J. Z. Hearon, *Kinetics of Intact Cells*, University of Vermont, February 2, 1955; Harvard Medical School, February 4, 1955.

W. C. Sangren, *Interface Problems for One, Two and Three Dimensions*, Tulane University, February 17, 1955; *Mathematics and High Speed Computers and the Problem of Interfaces in Mathematical Physics*, University of Miami, March 8, 1955; *Two and Three Dimensional Eigenvalue Problems*, University of Miami, March 9, 1955; Florida State University, March 10, 1955; *High Speed Computation of Eigenvalues*, University of Georgia, March 24, 1955.

S. G. Campbell, *Error Analysis and Numerical Methods*, Tuskegee Institute, February 28, 1955; University of Alabama, March 1, 1955; *Some Unsolved Problems on the Digital Computer*, University of South Carolina, March 24, 1955; *Classes on Non-linear Partial Differential Equations*, Duke University, April 19, 1955.

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

J. Z. Hearon, *Relative Roles of Diffusion and Reaction in Cellular Kinetics*, Naval Medical Research Institute, May 5, 1955.

A. W. Kimball, *Optimization Procedures in Chemical Processes*, Oak Ridge Chapter of the American Institute of Chemical Engineers, February 23, 1955.

A. W. Kimball and W. T. Burnett, Jr., *Sampling Methods for Screening Compounds in Radiation Protection Studies with Mice*, Radiation Research Society, New York City, May 16–18, 1955.

A. S. Householder, *On Solving Linear Algebraic Systems*, U.S. Naval Ordnance Laboratory, Silver Springs, Maryland, January 19, 1955; *The Oracle*, meeting of the Knoxville Mathematics Teachers, Knoxville, February 3, 1955; *On Solving Linear Algebraic Equations*, Purdue University, March 15, 1955; *Some Methods for Solving Linear Systems of Equations*, Battelle Memorial Institute, March 16, 1955; *Mathematics*

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by *Machinery*, annual meeting of the Mississippi Education Association, Jackson, Mississippi, March 17, 1955.

W. G. Howe, *Some Contributions to Factor Analysis*, eastern meeting of the Institute of Mathematical Sciences, Chapel Hill, North Carolina, April 22, 1955.

C. L. Bradshaw, *Career Opportunities in Mathematics*, career day for high school seniors, Tennessee Polytechnic Institute, March 21, 1955.

MEETINGS

Several members of the Panel attended the meeting of the Mathematical Association of America in Cookeville, Tennessee, on March 11, 1955. Those giving papers were as follows: A. S. Householder, *Mathematics for Computers*; C. L. Bradshaw, *Differential Equations with Interfaces Between Regions*; S. G. Campbell, *Computing Higher Mathematical Functions*; C. L. Gerberich, *Machine Computation of Definite Integrals*.

A. W. Kimball attended the joint meeting of the Institute of Mathematical Statistics and the Biometrics Society on April 22-23, 1955, in Chapel Hill, North Carolina.

LIST OF PUBLICATIONS

A. S. Householder, "Office Needs More Complex Computers Than Does Science," *The Office*, 41, No. 1, 82 (1955).

A. S. Householder, "Computers and Computation, Abroad and Here," *Computers and Automation*, 4, No. 2, 32 (1955).

A. S. Householder, "The Effect of Computers on the Training of Applied Mathematicians and Scientists," *Proceedings of the First Conference on Training Personnel for the Computing Field*, Wayne University Press, Detroit, 1955.

A. S. Householder, "Mathematics, the Schools, and the Oracle," *The Mathematics Teacher*, 48, 299-304 (1955).

A. S. Householder, *Bibliography on Numerical Analysis*, ORNL-1897 (June 6, 1955).

A. S. Householder, *On the Convergence of Matrix Iterations*, ORNL-1883 (May 18, 1955).

R. C. F. Bartels and A. C. Downing, Jr., "On Surface Waves Generated by Travelling Disturbances with Circular Symmetry," *Proceedings of the Second U.S. National Congress on Applied Mechanics*, pp 607-615, American Society of Mechanical Engineers, Ann Arbor, 1954.

J. Z. Hearon, "Note on the Theory of Mass Behavior," *Bull. Math. Biophys.* 17, 7-13 (1955).

J. Z. Hearon and J. B. Gilbert, "New Methods for the Calculation of Association Constants of Complex Ion Systems," *J. Am. Chem. Soc.* 77, 2594 (1955).

J. B. Gilbert, M. C. Otey, and J. Z. Hearon, "Association Constants for Cobalt-Glycine and Cobalt-Glycylglycine Complexes in Aqueous Solution," *J. Am. Chem. Soc.* 77, 2599 (1955).

D. J. Cavanaugh and J. Z. Hearon, "Kinetics of Acetylcholine Action on Skeletal Muscle," *Arch. intern. pharmacodynamie*, **100**, 68-78 (1954).

D. J. Cavanaugh, J. Harris, and J. Z. Hearon, "Enzyme Inhibition by Complexing of Substrates: Inhibition of Tyrosinase by Titanium Compounds," *J. Am. Chem. Soc.* **77**, 1531 (1955).

S. E. Atta and W. C. Sangren, "Calculation of Generalized Hypergeometric Series," *J. Assoc. Comp. Machinery*, **1**, No. 4, 170-172 (1954).

W. G. Howe, *Some Contributions to Factor Analysis*, ORNL-1919 (July 12, 1955).

F. W. Stallard, *Differential Systems with Interface Conditions*, ORNL-1876 (April 13, 1955).

EMPLOYEE CHANGES

F. R. Mance has joined the Panel as an Oracle operator. Three ORINS Fellows have joined the Panel; they are: T. W. Hildebrandt, from the University of Michigan; R. G. Cornell, from VPI; and R. D. Sheffield, from the University of Mississippi. W. G. Howe and F. W. Stallard, both from the University of North Carolina, completed their work as ORINS Fellows with the Panel. R. L. Plunkett, J. S. Rosen, and G. W. Medlin joined the Panel as research participants for the summer. M. D. George and R. C. F. Bartels both came to the Panel as temporary employees.

MATHEMATICAL RESEARCH AND SUBROUTINES

PROGRESS OF THE ORACLE SUBROUTINE LIBRARY

References: Mathematics Panel Semiannual Progress Reports, ORNL-1842, -1588, -1662, -1751; Mathematics Panel Quarterly Progress Reports, ORNL-1498, -1435

Background and Status. - The major effort with respect to subroutines has been channeled into several distinct areas, in accordance with the various purposes the subroutines are expected to serve. In the past, the main effort has been directed toward the production of adequate programs to perform as many of the necessary routine jobs as can profitably be carried out on the Oracle by such programs. The limit of feasibility in this direction has by no means been reached, or even approached, and a great deal remains to be done. However, particularly with the probability in the near future that all subroutines can be stored permanently on magnetic tapes and thus be made available to any programmer at any time in a matter of a few milliseconds, it has become at least equally important that subroutines which have been completed and tested be made available, along with all pertinent information about such subroutines, to all programmers.

In addition to the immediate problem of making paper tapes, codes, and descriptive writeups of all subroutines available as soon as the labor involved can be completed,

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there is the less pressing but more ultimately important job of making all subroutines instantly available on magnetic tape through the means of a really flexible compiler routine which would assemble not only the subroutines but, if desired, the entire program as well. The requirements of such a compiler are not difficult to state: it must be able to utilize information from both magnetic and paper tape, to handle a large number of "blocks" of code, subroutines, and constants, each block being of rather arbitrary size, and to assemble from these "blocks" an entire program on magnetic tape; it should also, if desired, print out a copy of the completed program. Further, regardless of its own internal complication, the routine itself should be easy to use.

The use of such a compiler presupposes that all subroutines (including the compiler itself) are available on magnetic tape, with a suitable classification number attached to each subroutine so that the compiler may be provided with the information it needs in order to load the given routine correctly. The suggested procedure is that all subroutines should be available on a single master tape and that each programmer should have available enough magnetic tape for his own use to permit storage of whatever material from the master tape he wants to use, in addition to his own codes. (Use of the master tape during computing would waste a tape drive and also leave open the possibility that an accidental write order would destroy the master tape.) Use of such a compiler is also a preliminary step toward automatic programming.

Many of the subroutines have had to be rewritten because of the imminent engineering changeover to an 8-12 transfer on partial substitution operations on the Oracle. However, the net effect here is beneficial, since no further changes will have to be made when using any of these programs with the 2048 word memory. In particular, the three-address packed floating point has been completely rewritten as an 8-32 packed floating point, with the consequence that all subroutines designed to go with the floating-point program have had to be rewritten.

In addition to the extensive amount of rewriting which is now going on, new floating-point trigonometric, logarithmic, exponential, n th root, and inverse trigonometric-function routines have been completed and are all now being used in production problems. A floating-point code which calculates (with full significance) $e^{-x} - 1$ for $x \geq 0$, as well as e^{-x} , depending upon which entrance to the routine is used, has been tested and is now being used in production problems. Such a code is particularly valuable in the evaluation of analytic solutions of linear differential equations with constant coefficients, where loss of significance for small argument is a serious problem. Floating-point programs have been written for evaluation of the Bessel I_0 , I_1 , J_0 , J_1 , K_0 , and K_1 functions. These codes are in the "debugging" stage. In addition, a program has been completed for solving the transcendental equation $n = xJ_1(x)/J_0(x)$, given n , and all these Bessel-function codes are now being incorporated into a single program which will calculate any of them.

The Graeffe method for solving arbitrary polynomials has been programmed and is now available for limited use, although testing of the program is not complete. Matrix inversion and equation-solving codes have been completed for arbitrary matrices. These programs use the internal memory if the matrix is no larger than 21×21 , and use the auxiliary magnetic-tape memory for larger matrices. Work is proceeding on the problem of calculating characteristic roots and vectors of arbitrary matrices. Several curve-fitting programs have been completed, and others are in the experimental stage.

New fixed-point trigonometric- and logarithmic-function codes have been completed and tested. The new trigonometric-function code is more than twice as fast as the fastest code previously available. The new logarithmic code is approximately three times as fast and half as long as the only comparable code which existed previously. (The trigonometric-function code requires 11.5 msec to calculate both $\sin x$ and $\cos x$; the $\ln x$ code requires 20 msec. This compares with 26 msec for the earlier trigonometric code and about 60 msec for the logarithmic code.)

Fourteen different Gaussian single numerical integration codes, using from 3- to 16-point Gaussian integration, at the discretion of the programmer, are being made available on magnetic tape. The floating-point Gaussian single integral will have to be entirely rewritten because of engineering changes in the Oracle. Trapezoidal and Simpson's rule automatic integration programs are now available, and additional formulas of the Newton-Cotes type will be programmed whenever time becomes available.

SERVICE ROUTINE FOR THE ORACLE

Participating Member of Panel: M. R. Arnette

Background and Status. – The service routine is used for solving a set of linear regression equations. It will invert the normal matrix, solve the normal equations, and give the residual sum of squares. The programmer must supply the order of the matrix and the elements of the upper triangular matrix augmented by the vector to be used in getting the solution.

This routine uses six blocks of magnetic tape for storage of code. The master code which stays in the electrostatic memory takes the input data (digital numbers), converts these numbers to correct machine form, and puts the entire augmented matrix into a fixed location. The master code also calls for a part of the code from the magnetic tape as each part is needed and keeps the magnetic tape correctly positioned. Calculation time for getting an inverse and the related functions of a matrix of order 14 is approximately 55 sec, not including punching of the answers.

This code has been tested by running a series of multiple regression problems for North Carolina State College.

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CALCULATION OF THE CHARACTERISTIC VALUES AND VECTORS FOR THE PRODUCT OF TWO SYMMETRIC MATRICES

Participating Members of Panel: M. R. Arnette, A. C. Downing

Background and Status. – Perturbation techniques will sometimes lead to secular determinantal equations of the form

$$|H - \lambda S| = 0 ,$$

where H and S are real symmetric matrices, and at least one of them, say S , is positive definite. Also, the characteristic vectors x , which satisfy the matrix equation

$$(1) \quad (H - \lambda S) x = 0 ,$$

are often desired. An equivalent problem is to find the characteristic values and vectors of the nonsymmetric matrix $S^{-1}H$.

Nonsymmetric matrices of this form have real characteristic values. In order to exploit this fact, the positive definite matrix S^{-1} may be factored by using its characteristic values and vectors. Thus, an orthogonal matrix, P , and a real diagonal matrix, D , may be found such that

$$S^{-1} = P^T D^2 P = (DP)^T (DP) = U^T U .$$

Introducing an auxiliary vector ξ defined by the relation

$$(2) \quad x = U\xi ,$$

and multiplying Eq. 1 on the left by U^T gives

$$(3) \quad U^T(H - \lambda S) U\xi = (U^T H U - \lambda I) \xi = 0 .$$

This is the familiar characteristic value and vector problem, with a symmetric matrix $U^T H U$. Once the λ 's and the vectors, ξ , have been obtained, the desired proper vectors x may be obtained from Eq. 2.

A routine for solving this problem has been prepared for the Oracle and has been used in several Laboratory problems. This routine makes use of the Oracle subroutines for calculating the proper vectors of symmetric matrices.

MULTIPLE LINEAR REGRESSION

Origin: Mathematics Panel

Participating Members of Panel: C. L. Gerberich, J. Z. Hearon, A. W. Kimball

Background and Status. – An attempt is being made to set up a general-purpose system to solve the large number of problems coming to the Mathematics Panel that are of a data-fitting nature. This system would fit the data in the following way:

$$F = a_1 x_1 + a_2 x_2 + a_3 x_3 + \dots + a_n x_n ,$$

where the a_i 's are the coefficients wanted. The x_j 's are variables believed to influence the value of the F in the range considered. In the case of an ordinary polynomial fit, $x_i = x^{i-1}$. For a two-dimensional problem, $x_i = f_i(x) g_i(y)$.

Let F_α ($\alpha = 1, 2, \dots, m$) be a random variable with the expected value

$$\mathcal{E}(F_\alpha) = \alpha_0 x_{0\alpha} + \alpha_1 x_{1\alpha} + \dots + \alpha_n x_{n\alpha}.$$

If matrix notation is used,

$$F = \begin{pmatrix} F_1 \\ F_2 \\ \vdots \\ F_m \end{pmatrix}, \quad X = \begin{pmatrix} x_{01} & x_{11} & x_{21} & \cdots & x_{n1} \\ x_{02} & x_{12} & x_{22} & \cdots & x_{n2} \\ \vdots & \vdots & \vdots & & \vdots \\ x_{0m} & & \cdots & & x_{nm} \end{pmatrix}, \quad \alpha = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}.$$

The so-called observation equations are

$$X\alpha = f,$$

and if $m > n + 1$, there are more equations than unknowns. Hence a is determined such that

$$(F - Xa)^T (F - Xa)$$

is a minimum. This leads to the normal equations

$$Ba = g,$$

where $B = X^T X$, $g = X^T f$, and a is said to be a least-squares estimate of α . If B is positive definite, the estimate is given by

$$a = B^{-1}g.$$

It is hoped that built-in statistical information about the fit will be programed into the code, such as total sum of the squares ($F^T F$), the reduction due to the regression ($a^T g$), the residual sum of the squares ($F^T F - a^T g$), and the degree of correlation of the coefficients. Although this is basically a magnetic-tape problem, the greater part of it has been coded and used as a paper-tape problem, with a fair amount of success.

NONLINEAR LEAST-SQUARES FIT

Origin: W. C. Sangren, Mathematics Panel

Participating Member of Panel: N. D. Given

Background and Status. - A program to fit experimental data or results of Oracle reactor calculations to the equation

$$\lambda(b) = \lambda_0 + ab^\alpha + bb^\beta$$

is being tested, with special emphasis on speeding convergence and guaranteeing a minimum for the sum of the squares of the differences. At this time, no conclusions have been reached.

CONVERGENCE AND STABILITY CRITERIA FOR NUMERICAL SOLUTIONS
OF HYPERBOLIC SYSTEMS OF EQUATIONS

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

Background and Status. — It is well known that the solutions of finite difference equations may be approximate solutions to problems involving partial differential equations. In general, the question of how good these solutions are remains largely unanswered.

A first-order linear system of equations of the form

$$(1) \quad U_t = AU_x + BU,$$

where U denotes the vector of dependent variables, and A and B are matrices independent of U , is said to be hyperbolic if there exists a real matrix T such that

$$TAT^{-1} = D$$

is a real diagonal matrix. Lax and Keller¹ have presented a finite difference scheme for solving such systems numerically. Moreover, they have been able to prove the convergence and stability of such solutions, provided the classical condition of Courant, Friedrichs, and Lewy is satisfied. For the staggered grid used by Lax and Keller, this condition states that the ratio of grid spacings in the t and x directions must satisfy the inequality

$$(2) \quad \frac{\Delta t}{\Delta x} \leq \frac{1}{2d},$$

where d is the absolute value of the numerically largest element of the diagonal matrix D . However, the convergence criteria given by them must be modified in one essential respect.

Let E be the error vector which represents the difference between the true solution U and the numerical solution, and let $\|E_n\|$ represent a suitable measure of the magnitude of this error at the n th time step in the numerical procedure. Then it can be shown, by applying the methods of Lax and Keller, that for a fixed value of $n \cdot \Delta t = T$, the error satisfies the inequality

$$(3) \quad \|E_n\| \leq \|E_0\| e^{bT} + \frac{e^{bT} - 1}{b} \left(\alpha \frac{\overline{\Delta x}^2}{\Delta t} + \beta \Delta t + \gamma \overline{\Delta x}^2 \right),$$

where α , β , γ , and b are constants depending upon a suitable norm for U_{xx} , U_{tt} , and B . However, it follows from inequality 2 that

$$4d^2 \Delta t \leq 2d \Delta x \leq \frac{\overline{\Delta x}^2}{\Delta t}.$$

Hence, if the initial values are exact (so that $\|E_0\| = 0$) and if the Courant, Friedrichs, and Lewy condition is satisfied, then the criterion for the convergence of the numerical

¹P. D. Lax and J. B. Keller, *The Initial and Mixed Initial and Boundary Value Problem for Hyperbolic Systems*, LAMS-1205 (Feb. 1, 1951).

solution to a solution of the system of partial differential equations (1) is that $\overline{\Delta x}^2/\Delta t$ tends to zero.

It is important to note that for fixed Δx (and practical considerations in using digital computers often impose a lower bound on the size of Δx) the upper bound of the magnitude of error is not necessarily decreased by decreasing the time spacing, Δt , alone. Indeed, it is easily seen from inequality 3 that for fixed Δx the optimum time spacing is such that $\Delta t/\Delta x = 1/2d$ or α/β , whichever is the smaller.

INVERSE CHARACTERISTIC VALUE PROBLEM

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

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Status. – The iterative procedure already described has been demonstrated to be a convergent process of first order. A second-order iteration has also been found.

TWO-REGION DIFFUSION-REACTION PROBLEM

Origin: J. Z. Hearon, Mathematics Panel

Participating Member of Panel: J. H. Vander Sluis

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – The two-region diffusion-reaction problem represents part of an extensive study of the influence of the spatial distribution of catalysts upon steady-state reaction rate in an open system. An incidental by-product of the general problem is an ensemble of exact solutions which can be used to establish the range of validity of certain approximate methods for solving multiregion problems. The three cases previously discussed have been coded for the Oracle. The code accepts values of the parameters and punches out concentration profiles and total reaction rates. In addition, the following problem has been coded. Let $k = k_1$ in the central region, $k = k_2$ in the outer region (cf. Eq. 1, p 34, above ref.), where the k_i are related in a prescribed manner to the total rate constant for the uniform case (Eq. 3, p 34, above ref.). Then the reaction rates in the two regions are

$$R_1 = 4\pi DA(a_1 r_1 \cosh a_1 r_1 - \sinh a_1 r_1) ,$$

$$R_2 = \frac{4\pi Dbr_0^2}{\Delta} [\alpha_1 \cosh \alpha_1 r_1 (\alpha_2 r_0 \cosh \lambda - \sinh \lambda - \alpha_2 r_1) + \alpha_2 \sinh \alpha_1 r_1 (\alpha_2 r_0 \sinh \lambda - \cosh \lambda + 1)] ,$$

where

$$A = \frac{br_0^2 \alpha_2}{\Delta} ,$$

$$\lambda = \alpha_2 (r_0 - r_1) ,$$

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$$\Delta = \alpha_1 \cosh \alpha_1 r_1 [br_0 \sinh \lambda + D(\alpha_2 r_0 \cosh \lambda - \sinh \lambda)] \\ + \alpha_2 \sinh \alpha_1 r_1 [br_0 \cosh \lambda + D(\alpha_2 r_0 \sinh \lambda - \cosh \lambda)] , \\ \alpha_i^2 = \frac{k_i}{D} ,$$

and the other quantities have been defined in the reference. A complete parameter study is being conducted on the functions R_i .

SELECTIVITY OF ION-EXCHANGE RESINS

Origin: G. E. Myers, Chemistry Division

Participating Members of Panel: C. L. Gerberich, J. Z. Hearon, A. W. Kimball

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – Computation of selectivity requires evaluation of the integral

$$- \int_0^y \frac{1}{m^2} \left[\frac{\partial m(x, \xi)}{\partial x} \right] d\xi = I(x, y) ,$$

where $m(x, y)$ is the total molality, x is the mole fraction of one member of the ion pair, and $y = -\ln a_w$ (cf. ref. p 36). In order to avoid the two-stage fitting procedure previously employed, it was proposed to fit the surface $1/m = g(x, y)$ and compute the integrand as $\partial g / \partial x$. Satisfactory fits were not obtained. At present, fits of the surface $m = f(x, y)$, where f is a general cubic polynomial, are being attempted by employing the multiple-regression code described in another section (cf. "Multiple Linear Regression," this report). Consideration is being given to improving the computed value of $1/m^2$ by employing a weighted fit and to computing the standard deviation of $I(x, y)$ from the variances and covariances of the parameters in $f(x, y)$.

TWO-DIMENSIONAL, TWO-REGION REACTOR CALCULATIONS

Participating Members of Panel: C. L. Bradshaw, W. C. Sangren

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – Work has been continued on the two-dimensional, two-region reactor problem. More refined difference approximations to the differential equations

$$(1) \quad \nabla^2 \phi + B^2 \phi = 0$$

and

$$(2) \quad \nabla^2 \phi - K^2 \phi = 0$$

have been made. Equation 1 can be approximated to the fourth order by

$$(3) \quad \left(4 + \frac{B^2 b^2}{2} \right) (\phi_{i+1, j} + \phi_{i-1, j} + \phi_{i, j+1} + \phi_{i, j-1}) + (4B^2 b^2 - 20) \phi_{i, j} \\ + (\phi_{i+1, j+1} + \phi_{i-1, j+1} + \phi_{i+1, j-1} + \phi_{i-1, j-1}) = 0 .$$

A similar expression can be written for Eq. 2. A refined approximation for the vertical derivative between two regions can be taken as

$$(4) \quad \phi_x \cong \left(\frac{1}{3} b + \frac{B^2 b^2}{12} \right) (\phi_{i+1,j} - \phi_{i-1,j}) + \frac{1}{12b} (\phi_{i+1,j+1} + \phi_{i+1,j-1} - \phi_{i-1,j+1} - \phi_{i-1,j-1}) = 0 .$$

This system of difference equations, with an appropriate set of boundary conditions, can be solved, and the resulting solution can be written as

$$(5) \quad \tan ax = -L \sin (xb) \left(\frac{4 + B^2 b^2 + 2 \cos \pi b^2}{4 - K^2 b^2 + 2 \cos \pi b^2} \right) ,$$

where

$$(6) \quad B^2 = \frac{20 - 4 \cos (xb) \cos \pi b - 8 \cos (xb) - 8 \cos \pi b}{b^2 [\cos (xb) + \cos \pi b + 4]} .$$

In Eq. 5 the quantity L is a constant, being a function of the mesh size (b) and the material composition of the two regions. Equation 5 has been solved for several variations in the parameters L and b . An example of the results is indicated below:

$$\nabla B^2 = B^2(\text{differential equation}) - B^2(\text{difference equation})$$

Second-order approximation: $b = 1/18$	+0.031
Second-order approximation: $b = 1/10$	+0.475
Fourth-order approximation: $b = 1/18$	-0.00054
Fourth-order approximation: $b = 1/10$	-0.0052

It should be noted that while the values of B^2 obtained as solutions of the second-order approximations are below the exact solution, the values obtained from the fourth-order approximation are above. This phenomenon has been justified by analytic considerations.

These results indicate that the improvements obtained by using the fourth-order approximations are such that there would be justification in complicating the difference equations in order to obtain the resulting reduction in the number of mesh points required to give a desired result.

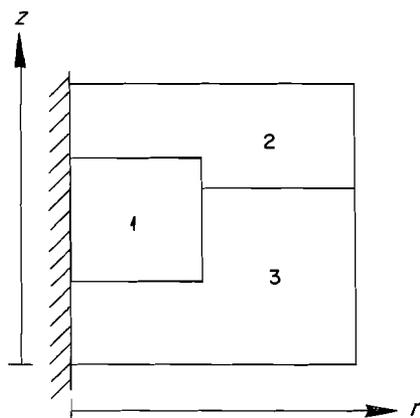
TWO-DIMENSIONAL, THREE-REGION, TWO-GROUP REACTOR CALCULATION

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

Participating Members of Panel: C. L. Bradshaw, W. C. Sangren

Background and Status. - A two-dimensional, three-region, two-group reactor problem is at present being coded for the Oracle. The geometry (cylindrical coordinates) of the problem is indicated below:

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Symmetry is assumed along the z axis. The numbers 1, 2, and 3 refer to the different regions.

The major problem, from the computational standpoint, is the solution of the large system of simultaneous algebraic equations which results when numerical methods are used for solving the elliptic partial differential equations describing the flux. This problem has been coded for the Oracle by using magnetic tapes. The size of the system of equations, and thus the number of mesh points, is practically unlimited.

The over-all problem is somewhat complicated because of the points which lie between regions – in particular, the corner points. Approximations have been made for the differential equations and boundary conditions that hold at these points.

PROBLEMS

ANALYSIS OF A SOLUBILITY EXPERIMENT

Origin: F. G. Tausche, Biology Division

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

Background and Status. – A comparison was made of the percentage of total liver protein soluble in two homogenizing fluids, 0.24 M sucrose and 0.1 M phosphate buffer. This was done with a group of normal rats and with a group which had received thyroxine daily for four days prior to killing.

The numbers of rats in each subgroup were not equal, and it was necessary to perform a disproportionate subclass number analysis of variance in order to evaluate the two main effects and the interaction. Both main effects were found to be significant

at the 1% level, but the interaction was negligible. Details of the experiment may be found in the last progress report of the Biology Division.¹

ANALYSIS OF DOSIMETRY DATA FROM THE ORNL 86-in. CYCLOTRON

Origin: C. W. Sheppard and M. Slater, Biology Division

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

Background. — During the period from August 1952 to September 1954, Biology Division personnel made extensive use of the ORNL 86-in. cyclotron to investigate the biological effects of fast neutrons. Some of these experiments were performed on a "crash" basis to obtain biological data so that effects could be predicted for optimum placing of material in nuclear detonation experiments. This early work was, on the whole, successful, and, in general, the fluctuations in the resulting data suggested that a valid semiquantitative experiment could be performed. Later, however, it appeared that there was a significant systematic error of 20 to 30% in the calibration, so several months were devoted in the spring and summer of 1954 to investigating the situation. The two principal factors were defective ion collection at high intensities and large-scale deflections and "aging" effects in the tissue-equivalent ion chambers. Sufficient data were obtained to correct for these effects, and, at the same time, biological experiments were performed in the later period to provide an additional check on the corrected results from the "crash" phase of the work. The relative results between the cyclotron and the field tests were not affected, since the field data were based on cyclotron calibrations. In the course of the later investigation, the situation became quite consistent, and, in addition, useful information was obtained, such as the successful comparison of tissue-equivalent ion chambers with the Hurst proportional counter system of dosimetry. It was therefore felt that perhaps the semiquantitative early results could be combined with the later observations to give more precise data and that publishable results might be obtained. Before such a decision could be made, it was necessary to analyze all the data statistically to avoid the possible effect of personal bias.

In the course of these experiments, more than 1000 physical observations had been obtained, plus considerable supporting data, such as x-ray calibrations of ion chambers, barometer and temperature readings, etc. A monitor counter had been used to control biological exposures, and it had been frequently calibrated against ion chambers and other instruments. In the later work it was continually checked against a standard neutron source. For periods of several months the results were highly consistent, and, also, at times, repeated measurements over periods of a few hours gave highly reproducible results. Nevertheless, at other times, drifts occurred in the dose per count, and late in the investigation sudden fluctuations began to develop. It was hoped,

¹F. G. Tausche and N. G. Anderson, *Biol. Semiann. Prog. Rep. Feb. 15, 1955*, ORNL-1863, p 76.

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therefore, that analysis of the data would permit a better evaluation of the probable effects of these disturbances on the biological findings.

Status. — In the first part of the analysis, corrections were made to the ion-chamber readings for factors which were known to have an effect. These included corrections for intensity and scale deflection, for position of the chamber inside the exposure facilities, for drifts in the monitor which were detected by calibration against a standard source, and for various calibration constants. In many cases this required the fitting of second-degree surfaces in three-space to the data from several exploration experiments.

In the second part of the study, analyses of variance of corrected readings were performed and showed, uniformly, the existence of a significant day-to-day variation. Subsequently, it was possible to group the data into homogeneous sets so as to provide more accurate dose estimates than could be obtained from any one day.

Finally, selected biological data, chosen so as to provide a comparison of the behavior of the cyclotron during the early and late periods, were analyzed. In general, the agreement in biological results from experiments performed at different times and by different investigators was excellent.

The results of this study, including the details of the statistical analyses, have been written up and will be distributed as a memorandum to biologists who have used or will use the 86-in. cyclotron as a source of neutrons.

AN ESTIMATION PROBLEM CONCERNING RING-X CHROMOSOMES IN *DROSOPHILA MELANOGASTER*

Origin: C. W. Hinton, Biology Division

Participating Members of Panel: R. G. Cornell, A. W. Kimball

Background and Status. — Typically, ring chromosomes in *Drosophila melanogaster* experience no difficulty in mitotic divisions. This problem is concerned with a unique ring-X chromosome which is unstable, as shown by its frequent production of XO males, gynandromorphs, and lethals in ring-X over rod-X zygotes. The experimental aspects of this problem are discussed in a recent Biology Division report.²

At first each zygote nucleus contains one ring-X chromosome and one rod-X chromosome. During the subsequent divisions, any rod-X chromosome is duplicated once during each division, but any ring-X chromosome either may be duplicated normally or may form an anaphase bridge. Such a bridge may, in turn, either break or be eliminated without breakage. Breakage results in lethality, but elimination without breakage during a series of divisions gives either an XO male, if all the ring-X chromosomes are eliminated, or a gynandromorph if only part of the ring-X chromosomes which have been formed are eliminated. Let p denote the probability of bridge formation, $q = 1 - p$ the probability of normal duplication of the ring-X chromosome, x the probability that a

²C. W. Hinton, *Biol. Semiann. Prog. Rep. Feb. 15, 1955*, ORNL-1863, p 41.

bridge breaks once it is formed, and $y = 1 - x$ the probability that after a bridge is formed it will be eliminated without breakage. Now, the zygote may be examined after n divisions, and the proportions of X0 male, gynandromorph, lethal, and normal zygotes may be determined. From these proportions it is desired to estimate q and y .

The problem may be represented by using stochastic matrices, but a solution in closed form has not been found in this way. However, let $\pi_1, \pi_2, \pi_3,$ and π_4 be the probabilities after n divisions of obtaining a normal zygote, an X0 male, a gynandromorph, and a lethal zygote, respectively. Now, if the generating function

$$\prod_{j=1}^n [p(x + y) + q] 2^{j-1}$$

is considered, it is seen that π_1 equals the sum of all terms of the expansion which involve only powers of q . Thus

$$\pi_1 = \prod_{j=1}^n q 2^{j-1} = q^{\sum_{j=1}^n 2^{j-1}} .$$

Similarly, the sum of all terms in the expansion which contain an x represents the probability of a lethal. Hence,

$$\pi_4 = 1 - \prod_{j=1}^n (py + q) 2^{j-1} = 1 - (py + q)^{\sum_{j=1}^n 2^{j-1}} .$$

The generating function cannot be used to obtain π_2 or π_3 , but if A_k is taken as the probability of an X0 male being formed during the first k divisions for $k = 0, 1, 2, \dots, n$, the recurrence relationship will be

$$A_k = qA_{k-1}^2 + py ,$$

given that $A_0 = 0$. Thus

$$\pi_2 = A_n = py + p^2qy^2 + 2p^3q^2y^3 + 5p^4q^3y^4 + R$$

for $n > 3$, where R contains other terms of the form $(\text{a constant}) \cdot p^{k+1} q^k y^{k+1}$, with $k > 3$. Enough terms may easily be included in the expression for π_2 so that the desired two- or three-place accuracy may be obtained. Finally, π_3 may be derived by subtraction, for

$$\pi_3 = 1 - \pi_1 - \pi_2 - \pi_4 .$$

From these expressions for $\pi_1, \pi_2, \pi_3,$ and π_4 , maximum likelihood estimates of q and y may be found by using Fisher's score method. Since the expressions for the π 's involve n , this procedure would require that n be known, and, as yet, n has not been accurately determined. Therefore, calculation of estimates of q and y has been postponed until n is determined experimentally.

FORMULAS FOR THE MEAN AND THE VARIANCE OF EQUATIONAL SEPARATION
IN THE AXOLOTL

Origin: D. L. Lindsley, Biology Division

Participating Member of Panel: R. G. Cornell

Background and Status. — If r is taken as the number of chiasmata formed in a chromosome during meiosis, then the formula for S_r , the equational separation, is

$$S_r = \frac{2}{3} \left[1 - \left(-\frac{1}{2} \right)^r \right].$$

Assume that r has a Poisson distribution with parameter n equal to the map distance, and let $g(n)$ be the mean equational separation. Now, $f(r) = e^{-n} n^r / r!$ for $r = 0, 1, 2, \dots$,

and $g(n) = \sum_{r=0}^{\infty} S_r f(r)$. Hence

$$\begin{aligned} g(n) &= \sum_{r=0}^{\infty} \frac{2}{3} \left[1 - \left(-\frac{1}{2} \right)^r \right] \frac{e^{-n} n^r}{r!} \\ &= \frac{2}{3} \sum_{r=0}^{\infty} \frac{e^{-n} n^r}{r!} - \frac{2}{3} \sum_{r=0}^{\infty} \left(-\frac{1}{2} \right)^r \frac{e^{-n} n^r}{r!} \\ &= \frac{2}{3} \left[1 - e^{-n} \sum_{r=0}^{\infty} \frac{(n/2)^{2r}}{(2r)!} + e^{-n} \sum_{r=0}^{\infty} \frac{(n/2)^{2r+1}}{(2r+1)!} \right] \\ &= \frac{2}{3} \left[1 - e^{-n} \left(\cosh \frac{n}{2} - \sinh \frac{n}{2} \right) \right] \\ &= \frac{2}{3} \left[1 - e^{-n} \left(e^{-n/2} \right) \right] \\ &= \frac{2}{3} \left[1 - e^{-3n/2} \right]. \end{aligned}$$

Furthermore, the expected value of S_r^2 is

$$\begin{aligned} E(S_r^2) &= \sum_{r=0}^{\infty} S_r^2 \cdot f(r) \\ &= \sum_{r=0}^{\infty} \left\{ \frac{2}{3} \left[1 - \left(-\frac{1}{2} \right)^r \right] \right\}^2 \frac{e^{-n} n^r}{r!} \\ &= \frac{4}{9} \sum_{r=0}^{\infty} \left[1 - 2 \left(-\frac{1}{2} \right)^r + \left(-\frac{1}{2} \right)^{2r} \right] \frac{e^{-n} n^r}{r!} \\ &= \frac{4}{9} \left[1 - 2e^{-n} \left(\cosh \frac{n}{2} - \sinh \frac{n}{2} \right) + \sum_{r=0}^{\infty} \frac{e^{-n} (n/4)^r}{r!} \right]. \end{aligned}$$

However,

$$\sum_{r=0}^{\infty} \frac{e^{-n(n/4)^r}}{r!} = e^{-3n/4} .$$

Therefore

$$\begin{aligned} E(S_r^2) &= \frac{4}{9} \left[1 - 2e^{-n} \left(\cosh \frac{n}{2} - \sinh \frac{n}{2} \right) + e^{-3n/4} \right] \\ &= \frac{4}{9} \left(1 - 2e^{-3n/2} + e^{-3n/4} \right) . \end{aligned}$$

Hence, the variance of S_r , given by $E(S_r^2) - g^2(n)$, is equal to

$$V(S_r) = \frac{4}{9} \left(e^{-3n/4} - e^{-3n} \right) .$$

ESTIMATION OF CYCLE LENGTH DURING SPERMATOGENESIS IN THE 101 × C₃H HYBRID MOUSE

Origin: E. F. Oakberg, Biology Division

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

Background and Status. - Male mice were exposed to 100 r of x rays and were killed at times after irradiation varying from 24 hr to 38 days. From cross sections of the testis, individual tubules in stage VII were scored for the presence of resting primary spermatocytes, primary spermatocytes in pachytene, spermatids, and spermatozoa. Four mice were killed at each time interval and for each cross section, and 20 tubules from each mouse were scored. In addition, for the first two cell types, actual cell counts were made. The four different types of cells disappear from the tubules during different periods after irradiation in the order listed above. Beginning at about 25 days, the spermatids reappear, and at 34 days the spermatozoa reappear.

At first it was thought that the disappearance curves in terms of mean number of cells per tubule would be of the same shape for each type of cell but simply displaced along the time axis. This point was checked by fitting curves to the two cell types for which cell counts were available, and it was found that resting primary spermatocytes disappear less rapidly than primary spermatocytes in pachytene. The same sort of check was then made on the presence-absence criterion, and it was found that no one function would fit all four disappearance curves.

Accordingly, different functions were fitted to each disappearance curve, and for each cell type the LD₅₀ (time at which 50% of the tubules contain at least one of the cell type being scored) was estimated. Then if T_i is the LD₅₀ for the i th cell type, taken in the order of its disappearance, the equation

$$T_i = \alpha + (i - 1)\beta$$

provides an estimate of the cycle length β , when fitted to the estimated LD_{50} 's. A weighted regression of this type was carried out and resulted in an estimate of the cycle length of 8.57 days, with a standard error of 0.38 day. An estimate of 8.70 days, with a standard error of 0.35 day, was obtained in a similar manner from the repopulation data. The two estimates are in good agreement. Details of this experiment may be found in another semiannual report.³

**A COMPONENTS-OF-VARIANCE ANALYSIS OF MAST CELL COUNTS
IN X-IRRADIATED RATS**

Origin: F. P. Conte, Biology Division

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

Reference: Mathematics Panel Quarterly Progress Report, ORNL-1232

Background and Status. – As part of a study of the role of mast cells in the radiation injury syndrome, rats were exposed to various doses of x rays, and slides were prepared from the mesentery region on each of several days after irradiation. Multiple counts of mast cells were made from each slide. An evaluation of the effects of dose and time after irradiation was the primary purpose of the analysis, but since this was the first experiment of a series, information was also requested on optimum values for the number of animals per treatment combination, the number of slides per animal, and the number of counts per slide.

As a model for the analysis of variance it was assumed that

$$y_{ijklm} = M + D_i + T_{ij} + A_{ijk} + S_{ijkl} + C_{ijklm}$$

($i = 1, \dots, n_i; j = 1, \dots, n_{ij}; k = 1, \dots, n_{ijk}; l = 1, \dots, n_{ijkl}; m = 1, \dots, n_{ijklm}$),
where

y_{ijklm} = m th count from the l th slide on the k th animal sacrificed at the j th time after irradiation by the i th dose,

M = average over-all mast cell count,

D_i = constant effect due to i th dose,

T_{ij} = constant effect due to j th time at the i th dose,

and where A_{ijk} , S_{ijkl} , and C_{ijklm} are random variables, normally and independently distributed with zero expectations and variances σ_A^2 , σ_S^2 , and σ_C^2 , representing the components of error attributable to animals, slides, and counts, respectively. In general, the n 's within a subclass were not equal, and it was necessary to compute the expected values of the analysis of variance mean squares in terms of the n 's, as described in the reference (cf. p 9). After the analysis of variance was computed, the components of variance were estimated to be

³E. F. Oakberg and R. L. DiMinno, *Biol. Semiann. Prog. Rep. Feb. 15, 1955*, ORNL-1863, p 59.

$$\sigma_A^2 = 385.6 ,$$

$$\sigma_S^2 = 94.7 ,$$

$$\sigma_C^2 = 122.4 ,$$

and the average mast cell count was 55.9. It is seen immediately that the largest component of error was contributed by the animal variation and that the smallest was contributed by variations from slide to slide on the same animal.

With this information it is possible to say something about optimum numbers of animals, slides, and counts. The variance of a mean obtained from γ counts on each of β slides from each of α animals is given by

$$\frac{\sigma_A^2}{\alpha} + \frac{\sigma_S^2}{\alpha\beta} + \frac{\sigma_C^2}{\alpha\beta\gamma} .$$

Clearly, any increase in the number of animals will decrease the contribution of all components of error, an increase in the number of slides will affect only the last two components, and an increase in the number of counts decreases only the contribution of that component. In addition, since the animal component was the largest, it was recommended that as many animals as feasible be used and that much less emphasis be placed on slide and count numbers. A second experiment essentially confirmed these results and yielded standard errors in the vicinity of 5 to 10%.

FITTING OF ULTRAVIOLET DOSE-HATCHABILITY DATA IN *HABROBRACON JUGLANDIS* (ASHMEAD)

Origin: R. C. von Borstel, Biology Division

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

Background and Status. – Irradiation of *Habrobracon* unfertilized eggs with ultraviolet rays may be done from either the convex or the concave side of the egg. The nucleus is located on the convex side, so that irradiation on the concave side inflicts damage only on the cytoplasm. Since the nucleus is, in general, more sensitive to radiation, the LD₅₀ for convex irradiation is only about 180 ergs/mm², whereas for concave irradiation it is in the vicinity of 1600 ergs/mm². These responses are measured in terms of the per cent of hatchability of the unfertilized eggs.

Certain aspects of the shapes of the hatchability curves remain unexplained. The curve resulting from concave irradiation follows the usual multihit survival form,

$$y = 1 - (1 - e^{-kD})^n ,$$

where y is the proportion of eggs hatching, D is the dose, and k and n are fitted constants. The constant n in this model is the number of sensitive units, all of which must be inactivated in order for hatching to be prevented. The data indicate that n is a large

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number, probably in excess of 1000, and this is what would be expected for cytoplasmic irradiation.

On the other hand, irradiation from the convex side, which inflicts primarily nuclear damage, yields a hatchability curve which clearly does not follow the simple multihit law. At first it appeared that there were two groups of units in the nucleus, one highly sensitive to radiation and one less sensitive. Since the unfertilized egg is a haploid, this would imply that the data should be representable by the sum of two single-hit curves, that is, the sum of two exponentials. When this fit was attempted, the chi-square test indicated clearly that the fit was a poor one. Subsequently, fits involving sums of single and double hit terms were attempted but were not successful.

One further approach is, perhaps, worth investigating. It is conceivable that the nuclear damage curve is multihit in nature but that hatchability can be prevented whenever a or more units are inactivated, where $a < n$. The theoretical curve representing this model presents a much more difficult fitting problem. Let $p = e^{-kD}$ be the probability that a sensitive unit is not inactivated after being exposed to a dose D . Then the probability that a or more units are inactivated is

$$\sum_{r=a}^n C_r^n p^{n-r} q^r ,$$

and the hatchability y would be given by

$$y = \sum_{r=0}^{a-1} C_r^n (1 - e^{-kD})^r (e^{-kD})^{n-r} .$$

It is well known that this partial sum can be represented as an incomplete beta function, and, when suitable data are available, an attempt will be made to fit this function.

ENERGY ABSORPTION FROM NEUTRONS AND GAMMA RAYS

Origin: M. Slater, Biology Division

Participating Members of Panel: J. Z. Hearon, J. H. Vander Sluis

Background and Status. -- In this problem it was desired to have calculated the energy absorbed per gram of material per incident neutron or photon. In particular, it was desired to have the ratio of the energy absorbed in a given material to that absorbed in air and in tissue for the purpose of evaluating the various materials as dosimeters. Calculations were made for 12 elements and 8 compounds at 20 energy levels. For neutrons, absorption coefficients, mean free paths, dose (for elements), dose due to each element in a compound, and total dose were calculated. For gamma rays, absorption coefficients, dose (for elements), proportion of the dose due to each process (Compton, photoelectric, and pairing), dose due to each element and each process in a compound, and total dose were calculated. This problem could have been considered as a hand calculation, except for the tremendous amount of information desired (10,000

numbers). For this reason an interpretive routine for simplified coding was used in setting up this problem for the Oracle. The results have been given to the originator.

URANIUM DISTRIBUTION AND EXCRETION STUDIES IN MAN

Origin: S. R. Bernard, Health Physics Division

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

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Status. – In connection with this problem, an Oracle code for the least-square fitting of data, with associated weights, to the sum of exponentials was required.

The minimizing equations of the function

$$V(a, \lambda) = \sum_{i=1}^N W_i \left(y_i - \sum_{K=1}^M a_K e^{-\lambda_K + i} \right)^2$$

were solved in a straightforward way. With initial estimates of the λ 's given, the equations $\partial V / \partial a_K = 0$, $K = 1, 2, \dots, M$, were solved for the a 's. With these estimates for the a 's, each equation, $\partial V / \partial \lambda_K = 0$, was solved for λ_K by Newton's method. As each new estimate of a given λ_K was obtained, it was used in obtaining the remaining λ 's. To carry out additional iterations, the procedure was then repeated.

The present code allows $N \leq 50$, $M \leq 6$. The order of computing the λ_K 's and the number of Newton iterations to be carried out per λ_K may be specified. The arithmetic of the program is packed floating point.

ESTIMATION OF DAMAGE TO THE GASTROINTESTINAL TRACT

Origin: W. S. Snyder, Health Physics Division

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

Background and Status. – The damage to a portion of the gastrointestinal tract due to the ingestion of a radioactive isotope is influenced by the radioactive decay rate of the isotope and of the daughters which may replace it, and also by the partial or complete elimination of the isotope and daughters from the gastrointestinal tract by absorption into the blood stream. The Oracle was used to compute the damage to the gastrointestinal tract, taking account of biological elimination. For this computation, the gastrointestinal tract was considered to be composed of four regions: the stomach, small intestine, upper large intestine, and lower large intestine. It was assumed that one atom of a certain isotope was ingested and that this atom and its daughters moved through the gastrointestinal tract, spending 1 hr in the stomach, 4 hr in the small intestine, 8 hr in the upper large intestine, and 18 hr in the lower large intestine. It was assumed that biological elimination occurred at a constant rate during the 4-hr period in the small intestine and that no absorption occurred in the other three regions.

For a parent isotope having k daughters, the number of atoms of each kind as a function of time is determined by the solution of the following differential equations:

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In the regions where no absorption occurs –

$$\frac{dN_0(t)}{dt} = -\lambda_0^r N_0(t) ,$$

$$\frac{dN_i(t)}{dt} = \lambda_{i-1}^r N_{i-1}(t) - \lambda_i^r N_i(t) , \quad i = 1, 2, \dots, k ,$$

where $N_i(t)$ is the number of atoms of the i th daughter at time t , and λ_i^r is the radioactive decay constant for the i th daughter. The subscript 0 refers to the parent isotope.

In the region where absorption occurs –

$$\frac{dN_0(t)}{dt} = -\lambda_0^r N_0(t) - \lambda_0^b N_0(t) ,$$

$$\frac{dN_i(t)}{dt} = \lambda_{i-1}^r N_{i-1}(t) - \lambda_i^r N_i(t) - \lambda_i^b N_i(t) ,$$

where λ_i^b is the biological elimination constant based on experimental values of the fractional amount of an isotope absorbed into the blood stream. If f_i is this experimental value, then λ_i^b is found by solving

$$f_i = e^{-\lambda_i^r} \int_0^4 \lambda_i^b e^{-(\lambda_i^b + \lambda_i^r)t} dt .$$

The initial values for both systems are

$$N_0(0) = 1 ,$$

$$N_i(0) = 0 , \quad \text{for } i = 1, 2, \dots, k .$$

The initial values in regions 2, 3, and 4 would then be the values of N_0 and N_i for the end of the previous region.

The values of the concentrations N_i , $i = 0, 1, \dots, k$, were calculated at hourly intervals for approximately 100 different parent isotopes. Whenever a daughter isotope was stable or had a half life very large compared with the total time of 31 hr spent in the gastrointestinal tract, the chain was terminated. The longest chains considered had six daughter isotopes.

The rem dose as a function of time was then calculated by using the values of the concentrations $N_i(t)$:

$$D_{\text{rem}} = \frac{T}{2M} \sum_{i=0}^k N_i(t) \lambda_i^r D_i ,$$

where D_i is the energy, weighted by the RBE, released by a disintegration, M is the mass of the content of the section of the gastrointestinal tract considered, and T is the time of traversal through that section.

As a final result, the rem doses were used to calculate the maximum permissible concentrations of each parent isotope, in both air and water, which would result in an allowed dose of 0.3 rem per week.

This problem was completed.

DAMAGE TO TISSUE FROM NEUTRON IRRADIATION

Origin: W. S. Snyder and J. Neufeld, Health Physics Division

Participating Members of Panel: N. M. Dismuke, J. H. Vander Sluis

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background. – As stated in the reference, the National Committee on Radiation Protection has recommended that the RBE factors (relative biological effectiveness of the various recoil atoms in producing tissue damage) used in computing damage be made a function of average specific ionization. Previously, a constant value of RBE has been used for each type of recoil. To carry out the recommendation and at the same time to anticipate improvements in the knowledge of RBE as a function of specific ionization, the first four moments of average energy loss to tissue per incident neutron will be tabulated as a function of penetration in tissue and of type of recoil produced. The damage curves will then be obtained by polynomial approximations in terms of the tabulated moments. For a detailed description of the problem, see the memorandum by Snyder and Neufeld.⁴

Status. – The program breaks down into two Monte Carlo problems. Neutron histories are calculated in the first of these, and from the histories are tabulated the gamma rays produced by the $H(n,\gamma)$ reaction and the moments of energy transmitted to tissue through protons and heavier recoil atoms. This program allows the tissue-slab model to contain a column of bone. Also, the program allows the alternative of a plane source or a beam at any specified angle. The code for this part is being debugged.

The second problem⁵ begins with the gamma source tabulated in the first part and computes the gamma-ray contribution to the damage. This program was written for an earlier damage problem and can be used as it stands for a tissue slab. Modifications will have to be made to allow the column of bone to be included.

TEMPERATURE DEPENDENCE OF RESISTANCE

Origin: G. Ritscher, Instrumentation and Controls Division

Participating Member of Panel: C. P. Hubbard

Status. – An Oracle code was written to evaluate a polynomial expressing resistance as a function of temperature. A table of values was constructed for 500 values of temperature.

⁴W. S. Snyder and J. Neufeld, *Proposed Program for Computing the Rem Dose Due to Irradiation by Fast Neutrons* (unpublished memorandum).

⁵This program was written by C. D. Zerby of the Physics Division.

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BOND STRENGTHS OF ORGANIC MOLECULES

Origin: J. G. Burr, Chemistry Division

Participating Members of Panel: M. R. Arnette, A. C. Downing

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Status. – The technique chosen for solving the secular equation when the overlap matrix, $S_{\mu\nu}$, is not the identity matrix is described elsewhere in this report.

The π -electron densities for the ground state and for various ionized and excited states can be determined from the molecular orbitals. The calculation of these densities from the molecular orbitals requires the normalization of the principal vectors relative to the overlap matrix. If ϕ_i^j represents the j th component of the i th vector after normalization, then the electron densities are the diagonal elements of the matrix $P = (p_{ij})$, where

$$p_{ij} = \frac{1}{2} \sum_{k=1}^m N_k \phi_k^i \sum_{\nu=1}^n s_{j\nu} \phi_k^\nu + \frac{1}{2} \sum_{k=1}^m N_k \phi_k^j \sum_{\nu=1}^n s_{i\nu} \phi_k^\nu .$$

The summation over k represents a weighted sum of the diadic products. The choice of the weights N_k specifies the state of the molecule.

OSMOTIC COEFFICIENTS FOR ION-EXCHANGE RESINS

Origin: G. E. Myers, Chemistry Division

Participating Members of Panel: J. Z. Hearon, V. C. Klema, A. W. Kimball

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – The previously reported calculations on osmotic coefficients (cf. ref. p 38) were preliminary, and the fitting procedure that was employed has been improved in two respects: the nonlinear nature of the problem has been handled in a satisfactory manner, and, more important, the molality, m , which is determined subject to random error, has been fitted as a function of the equilibrium vapor pressure, which is assigned without sensible error. On this basis the appropriate function is

$$(1) \quad m = f(a, y) \frac{(ya_2 - a_3) + [(a_3 + ya_2)^2 + 4a_1y]^{1/2}}{2(a_1 + a_2a_3)} ,$$

where $y = k \ln a_w$ (cf. ref.), and the a_i are parameters to be estimated. Least-square estimates of the a_i were obtained by solving the system

$$(2) \quad (X^T X) \delta = X^T b ,$$

where the x_{ij} is $\partial f(a, y) / \partial a_j$ evaluated at some current estimate of the a_i , b is the column vector of differences between the observed and computed m 's, and δ is the column vector of corrections to the current estimates. The problem has been coded for the Oracle. The code accepts paired values of m and y and initial estimates of the a_i ; iterates on system 2 until $\delta^T \delta$ is less than a prescribed value; punches out the final a_i , the elements

of $(X^T X)^{-1}$, and the sum of squares of deviations, $b^T b$. Some 100 cases have been run, with satisfactory results returned to the originator, and the code is available for routine production.

FITTING CURVES TO SPECTRUM READINGS

Origin: C. Feldman, Chemistry Division

Participating Members of Panel: M. E. Fulmer, A. W. Kimball

Background and Status. – The best curve was obtained by a least-squares fit to the data from the spectrum readings. Twenty-five curves with seven points to each curve were fitted.

A TRIPLE INTEGRATION PROBLEM

Origin: H. Zeldes, Chemistry Division

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

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – Some modifications were made in the triple integrals referred to in the reference, and the new integrals were evaluated on the Oracle by using a standard Gaussian integration subroutine.

FOURIER INVERSION OF DIFFRACTION DATA

Origin: P. C. Sharrah and H. A. Levy, Chemistry Division

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

Background and Status. – X-ray diffraction data from liquid mercury were subjected to Fourier analysis in order to obtain the atomic radial distribution function. The integral

$$\int_0^{S_0} [af(S) - 1] S \sin RS \, dS$$

was evaluated for

$$R = 0, 0.1, 0.2, \dots, 10.0,$$

$$S_0 = 9.25,$$

$$S_0 = 11.95,$$

$$S_0 = 14.45,$$

$$a = 1.01, 1.00, \text{ and } 0.99.$$

The problem was done on the Oracle by using trapezoidal integration, and the results have been given to the originators.

SCATTERING BY A CYLINDRICAL SHELL WHICH SURROUNDS AN ABSORBING MEDIUM

Origin: H. A. Levy and P. C. Sharrah, Chemistry Division

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

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – The problem is concerned with the correction of neutron diffraction data for scattering arising from the sample container. The experimentally measured beam profile was treated. The function

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

was evaluated for $\phi = 0, 20^\circ, \dots, 180^\circ$ and for various values of B and $f(\cos \alpha)$.

The 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, M. E. Fulmer, V. C. Klema, W. C. Sangren

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background. - In this problem there are four given parameters as follows:

1. the subshell, M : five cases;
2. the gamma-ray energy, k : ten cases;
3. the atomic number, z : eight cases;
4. the multipole: ten cases of 2^L pole radiation;

<ol style="list-style-type: none"> a. five electric multipoles b. five magnetic multipoles 	$\left. \vphantom{\begin{matrix} a. \\ b. \end{matrix}} \right\} L = 1, 2, 3, 4, 5 .$
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The internal conversion coefficients for 2^L pole radiation are as follows:

1. electric radiation: $\beta_L(E)$,
2. magnetic radiation: $\beta_L(M)$.

These coefficients are given in terms of the coefficients $S_L(E)$ and $S_L(M)$. The quantities $S_L(E)$ and $S_L(M)$ are obtained from separate formulas given for each subshell in terms of the radial integrals R_1, R_2, R_3, R_4, R_5 , and R_6 . All these expressions are for particular values of k and z . The radial integrals depend on two parameters, κ and κ' . The subshell completely determines the value of κ' . The value of κ , as well as the value of L , is determined from the subshell. The absolute value of κ determines another parameter, λ . The radial integrals for each subshell are given in terms of $I_\sigma(\lambda, \kappa', \pm P)$ and $\tilde{I}_\sigma(\lambda, \kappa', \pm P)$ for $\sigma = L$ and $\sigma = L - 1$. The $I_\sigma(\lambda, \kappa', \pm P)$ and $\tilde{I}_\sigma(\lambda, \kappa', \pm P)$ are given in terms of $J_\sigma^{(n)}(\lambda, m, \pm P)$, where $m = |\kappa'|$, and $n = 0, 1, 2$. The $J_\sigma^{(n)}(\lambda, m, \pm P)$ are given as a sum over v (from 0 to σ) of the functions $H(\mu, \pm P)$, where $\mu = v - n$; $H_\lambda(\mu, \pm P)$ is a combination of many complex-valued functions.

The following subroutines were written for the complex-valued functions: (The Γ function in the complex plane employs an asymptotic expansion called Stirling's series.)

$$1. \log_e \Gamma(z) \sim z - \frac{1}{2} \log_e z - z + \frac{1}{2} \log_e (2\pi) + \sum_{m=1}^{\infty} \frac{(-1)^{m-1} B_m}{2m(2m-1) z^{2m-1}} ;$$

2. $\sin z = \sin x \cosh y + i \cos x \sinh y$ employs the series for $\frac{1}{2} \leq x < 1$ and $\frac{1}{2} \leq y < 1$ and the identities,

$$\sin^{i+1} x = 2 \sin 2^i x \cos 2^i x,$$

$$\cos 2^{i+1} x = 2 \cos^2 2^i x - 1,$$

$$\sinh 2^{i+1} x = 2 \sinh 2^i x \cosh 2^i x,$$

$$\cosh 2^{i+1} x = 2 \cosh^2 2^i x - 1;$$

3. $e^z = e^x (\cos y + i \sin y)$;
 4. $\ln z = \frac{1}{2} \ln (x^2 + y^2) + i \tan^{-1} y/x$;
 5. $(x + iy)^{a+ib} = e^{(a+ib) \ln(x+iy)}$;
 6. ${}_2F_1(\alpha_1 + i\beta_1, \alpha_2 + i\beta_2; \gamma_1 + i\delta_1; x + iy)$;
 7. complex arithmetic.

Since almost all the arithmetic is complex, the behavior of the numbers could not be determined. Therefore, it became necessary to use floating-point arithmetic in the programming of this problem.

Because there are similarities between subshells I and II and between III and IV, the problem was divided into three parts. Each of the three parts was programmed in three sections of code. The entire program employs the use of the magnetic-tape external memory.

Status. - Coefficients from subshells I and II have been obtained. The program for subshells III and IV has been written and is now being checked out. The program for subshell V has not been written.

LEAST-SQUARE FITTING FOR THE XENON CROSS SECTION

Origin: S. Bernstein, Physics Division

Participating Members of Panel: N. M. Dismuke, C. L. Gerberich, J. Z. Hearon, A. S. Householder, J. H. Vander Sluis; T. Arnette, Physics Division

Background and Status. - The set of constants $\vec{X} = (\Gamma_{n0}, \Gamma_{\gamma}, E_0, I_2, I_3, I_5, I_6, I_7)$ were determined by minimizing the function

$$V(\vec{X}) = \sum_{r=1}^7 V_r(\Gamma_{n0}, \Gamma_{\gamma}, E_0, I_r),$$

where

$$V_r = \sum_{i=1}^{p_r} W_i \left[\frac{Z_i}{I_r} - f(E_i; \Gamma_{n0}, \Gamma_{\gamma}, E_0) \right]^2.$$

The E_i values are not necessarily the same for the various run numbers, r . The weights depend on Z_i and I_r .

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The I_1 , the I_4 , and the Z_i 's are experimental measurements;⁶ the I_1 and I_4 measurements and the Z_i 's are independent. The function f , the Breit-Wigner⁷ total-cross-section formula, is given by

$$f(E_i; \Gamma_{n0}, \Gamma_\gamma, E_0) = \frac{b^2}{2\pi m} g \frac{\Gamma_{n0}}{\sqrt{E_0}} \frac{\Gamma_\gamma + \sqrt{E} \Gamma_{n0} / \sqrt{E_0}}{\sqrt{E} [(\Gamma_\gamma + \sqrt{E} \Gamma_{n0} / \sqrt{E_0})^2 + 4(E - E_0)^2]}$$

The fitting was carried out by a well-known iterative procedure.⁸ The minimizing equations of $V(\vec{X})$ were linearized by expanding in a Taylor series about \vec{X}_0 , the initial estimate of \vec{X} , and dropping terms above the first derivatives. The resulting set of eight linear equations was solved so that corrections could be applied to the initial estimates. Since the weights depend on the variances of some of the least-square parameters, the variance-covariance matrix had to be obtained for each iteration. The procedure was repeated until no significant changes occurred in the parameters or their variances.

The fitting was carried out for two values of g . For each g the final values of the least-square parameters were within a few per cent of the initial estimates; the changes in their variances were greater. Ten or twelve iterations were required.

SCATTERING OF X RAYS BY NEUTRON-IRRADIATED DIAMOND

Origin: H. C. Schweinler, Solid State Division

Participating Member of Panel: M. F. Todd

Background and Status. - To calculate the scattering of x rays by a neutron-irradiated diamond it was necessary to evaluate the functions

$$f^v(x, y, \epsilon) = \frac{2 + x^2 + y^2}{2(1 + x^2 + y^2)^2} [(A - 1)^2 + B^2]$$

and

$$f^i(x, y, \epsilon) = \frac{2 + x^2 + y^2}{2(1 + x^2 + y^2)^2} [(A + 1)^2 + B^2],$$

where f^v gives the vacancy scattering, and f^i gives the interstitial scattering; x , y are coordinates of position on a photographic plate, and ϵ gives the displacement of an atom.

$$\begin{aligned} A = & \cos \epsilon k(S_1 + S_2 + S_3) - \cos k(S_1 + S_2 + S_3) \\ & + \cos \epsilon k(S_1 - S_2 - S_3) - \cos k(S_1 - S_2 - S_3) \\ & + \cos \epsilon k(-S_1 + S_2 - S_3) - \cos k(-S_1 + S_2 - S_3) \\ & + \cos \epsilon k(-S_1 - S_2 + S_3) - \cos k(-S_1 - S_2 + S_3); \end{aligned}$$

⁶S. Bernstein, et al., *Phys. Quar. Prog. Rep. Dec., Jan., Feb. 1948-1949*, ORNL-325, p 6-68.

⁷S. Glasstone and M. C. Edlund, *The Elements of Nuclear Reactor Theory*, pp 27 and 56, Van Nostrand, New York, 1952.

⁸F. Garwood, *Biometrika* 32, 46 (1941).

B is equal to the same expression, with "sin" for "cos" throughout.

$$S_1 = \frac{x}{\sqrt{1+x^2+y^2}}, \quad S_2 = \frac{y}{\sqrt{1+x^2+y^2}},$$

$$S_3 = \frac{1}{\sqrt{1+x^2+y^2}} - 1, \quad k = \frac{\pi}{2} \frac{3.5675}{0.71069}.$$

The functions f^v and f^i were calculated over the ranges
 $x = 0(0.1)1$, $y = 0(0.1)1$, $\epsilon = 0.7(0.1)1.3$.

The problem was coded for the Oracle, and the results have been given to the originator.

A CONDUCTION-RADIATION PROBLEM

Origin: C. W. Cunningham, Aircraft Reactor Engineering Division

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

Background and Status. – Given a steady-state in-pile loop, the problem is to find the time-course of the temperature of the fuel and containing pipe (in particular, the time at which the inner wall of the pipe reaches its melting point) in the event of complete and sudden pump failure. With some geometric simplification, this problem was set up, and it was shown that, with conservative assumptions, the problem can be reduced to a three-region heat problem, with constant sources in two regions: standard interface conditions at one interface, and a radiation condition at the other. This idealized problem was solved by first-order finite difference equations. To assess the sensitivity of the final result to various assumptions, an extensive parameter study was made which revealed that assigning various values to the parameters had little effect. Results were returned to the originator.

HEAT TRANSFER AND PHYSICAL PROPERTIES IN A CIRCULATING-FUEL, CIRCULATING-MODERATOR REACTOR

Origin: J. O. Bradfute, Reactor Experimental Engineering Division

Participating Member of Panel: J. H. Vander Sluis

Background and Status. – This problem consisted of a parameter study from which temperature structure could be predicted in a circulating-fuel, circulating-moderator reactor system and from which pressure drops and pumping powers could be determined that would achieve 200-Mw heat extraction. The problem could be considered a hand calculation, except for the tremendous amount of information desired (20,000 numbers). For this reason an interpretive routine for simplified coding was used. The results have been given to the originator. A report on the results, by J. O. Bradfute and H. F. Poppendiek, is in preparation.

CALCULATION OF STRESS ANALYSIS IN PIPING SYSTEMS

Origin: M. I. Lundin, Reactor Experimental Engineering Division

Participating Member of Panel: E. C. Long

Background and Status. – A program has been prepared for the determination of stresses in three-plane piping systems. With input data describing all segments of a three-plane line, the coding first provides the coefficients, and sets up and solves a matrix for the end reactions and moments, taking into account both thermal expansion and anchor movements. These forces and moments are then converted into stresses at any point, in accordance with the Principal Stress Theory, which takes into account bending, loop, torsional, and lateral stresses in the pipeline. Calculation of deflections and rotations at any point for use in determining the requirements for pipe hangers and supports is also possible.

The Principal Stress Theory states that stresses are combined as follows:

$$S = \frac{1}{2} \left[S_l + S_c + \sqrt{4S_t^2 + (S_l + S_c)^2} \right] ,$$

where the pressure stress $S_p = P(D - t)/4t$, and the circumferential stress (loop stress) = $2S_p$; therefore the total longitudinal stress = $S_l = S_b + S_p$, and the torsional stress $S_t = C/2(M_t)$, where M_t is the torsional moment, and C is a constant.

The programming of this problem is complete, and the code is routinely in use on a production basis.

ESTIMATE OF APPLIANCE SATURATION BY CURVE FITTING

Origin: Tennessee Valley Authority

Participating Member of Panel: M. Hochdorf, Tennessee Valley Authority

Background and Status. – The number of consumers, C_j , using electric energy in the class interval from x_j through x_{j+1} kwhr is considered to consist of the sum of consumers in different overlapping homogeneous groups distinguished by the types of electrical appliances they use. The consumers in the individual groups are assumed to be normally distributed with respect to their electric energy consumption. If the total number of consumers in the i th group is N_i , the number in the group using electric energy in the class interval from x_j through x_{j+1} kwhr is

$$N_i \int_{(x_j - \bar{x}_i)/\sigma_i}^{(x_{j+1} - \bar{x}_i)/\sigma_i} \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt = N_i \phi_{ij} ,$$

where \bar{x}_i and σ_i are the mean and standard deviation, respectively, of the i th group. The total number of consumers in each class interval is then given by

$$\sum_i N_i \phi_{ij} = C_j .$$

Initial estimates of \bar{x}_i and σ_i are available. By using the method of least squares, the

linearly entering N_i are computed from a set of simultaneous equations with the side condition

$$\sum_i N_i = \sum_j C_j .$$

Least-squares solutions for improved \bar{x}_i and σ_i are then obtained by using Newton's method. The entire procedure is iterated until stable values for the parameters are obtained. Trials are being run to determine the number of parameters that will give a unique fit to C_j .

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, -1842

Background and Status. – The multigroup program, Eyewash, written for the Univac, has been used by ORNL for two reactor studies during the last six months. At present it has been made available to several other installations, including KAPL, NDA, Hanford, Argonne, the Babcock and Wilcox Co., Westinghouse, Brookhaven, and Wright-Patterson, in addition to the ANP and HR Projects of ORNL. A complete report on the program is in publication at present.⁹ Copies of the code and the Univac tapes are also available to any other groups desiring them.

NOMOGRAM FOR ORDERING-POINT CALCULATION

Origin: A. J. Cook, General Office Division

Participating Member of Panel: C. P. Hubbard

Status. – A nomogram was designed for General Stores to be used in determining the ordering-point quantity of any item according to the formula

$$Q = (1 + R) TC ,$$

where

Q = ordering-point quantity,

R = reserve, in per cent,

T = procurement time, in months,

C = consumption rate, in units per month.

The nomogram is now in use by General Stores.

⁹J. H. Alexander and N. D. Given, *A Machine Multigroup Calculation – The Eyewash Program for Univac*, ORNL-1925 (to be published).

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BUSINESS PROBLEMS ON THE ORACLE

Origin: G. E. Malone, Director's Division

Participating Members of Panel: N. D. Given, C. P. Hubbard

Background and Status. – Several business-type problems have been presented as possible routine calculations to be run periodically on the Oracle. Although it would certainly be desirable for these problems to be done automatically, it would be highly inconvenient with the present Oracle output system.

A program was prepared and tested that simulated the source-fission inventory system. The program read in the last month's ending inventory, processed it by a series of the month's transactions, and punched a new ending inventory tape. The nature of this typical problem necessitates much tape reading and punching by the machine, as well as the representation of all alphabetic data by some numerical code. For these reasons, it has been recommended that the writing of these programs, which process large volumes of data, be delayed until the output system is complete.

CRYSTAL STRUCTURE DETERMINATION OF PHOSPHORIC ACID HEMIHYDRATE

Origin: Tennessee Valley Authority

Participating Member of Panel: M. Hochdorf, Tennessee Valley Authority

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842, "Summation of a Double Fourier Series"

Background and Status. – Crystal structure determination of various compounds is one of the fundamental research activities carried on by the TVA's Division of Chemical Development at Wilson Dam, Alabama. The existing code given in the reference was used to obtain the double Fourier series summation, with intensities derived from x-ray diffraction as the coefficients.

"M" LINE CHARACTERISTICS – MATRIX SOLUTION

Origin: Tennessee Valley Authority

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

References: Mathematics Panel Semiannual Progress Reports, ORNL-1751, -1842

Status. – The matrix $Z = Z_1 - AF^{-1}B - DG^{-1}H$ was computed. The 36×36 matrix obtained from Z by deleting the first six rows and columns was inverted. Since Z is the real representation of a complex symmetrical matrix, the inversion was performed by partitioning the 36×36 matrix into its real and imaginary parts, $R + iX$. Both R and X are real, symmetrical, and of order 18. The real part of the inverse is given by $(R + XR^{-1}X)^{-1}$, and the imaginary part by $R^{-1}X(R + XR^{-1}X)^{-1}$. From Z , also, the 14×14 matrix, $Z'' = C_1 Z C_1^T$, was obtained. The 12×12 matrix remaining after deleting the first two rows and columns from Z'' was inverted. As a check, TVA obtained

the 12×12 matrix and its inverse on their a-c network analyzer by using a number of simplifying assumptions. Their answers compared favorably with the exact ones given by the Oracle. A paper on this problem by R. B. Shipley, M. Hochdorf, and M. Watson has been accepted for publication in *Transactions of the American Institute of Electrical Engineers*.