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UC-32 – Mathematics and Computers
TID-4500 (17th ed.)

MATHEMATICS PANEL
ANNUAL PROGRESS REPORT
FOR PERIOD ENDING DECEMBER 31, 1961

OAK RIDGE NATIONAL LABORATORY
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ADDENDUM TO ORNL-3264

G. J. Atta's name was inadvertently omitted from the list of participants under Programming and Programming Research on page 5. Please insert his name following D. E. Arnurius.

A S Householder

A. S. Householder

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ANNUAL PROGRESS REPORT

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

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OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
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Contents

Mathematics and Numerical Analysis

D. H. Clanton   Walter Gautschi   A. S. Householder

NUMERICAL INTEGRATION

As observed previously,[1] there is a close connection between numerical integration formulas which are exact if applied to trigonometric polynomials of given order and the (classical) formulas which are exact if applied to ordinary algebraic polynomials of given degree. The reason for this may be found in the following general fact.[2] Consider functionals

$$Lx = \beta_1 L_1 x + \ldots + \beta_{2p} L_{2p} x + L_{2p+1} x \,,$$

where β_λ are real parameters and L_λ are fixed linear functionals, continuous in the space $C^s\,[a,b]$ for some $s \geqq 0$, and satisfying $L_\lambda\, 1 = 0$ $(1 \leqq \lambda \leqq 2p + 1)$. Suppose there is a unique set, $\beta_\lambda = \beta_\lambda^0$, of the parameters such that $Lx = 0$ for every polynomial $x(t)$ of degree $\leqq 2p$. Then, if T is sufficiently large, there is also a unique set of parameters, $\beta_\lambda = \beta_\lambda(T)$, such that $Lx = 0$ for every trigonometric polynomial $x(t)$ of order $\leqq p$ having period T. Furthermore, $\beta_\lambda(T) \to \beta_\lambda^0$, as $T \to \infty$.

Functionals of the form

$$Lx = \sum_{\lambda=0}^{k} \left\{ \alpha_\lambda x[(k - \lambda)h] - h\beta_\lambda x'[(k - \lambda)h] \right\} \qquad (\alpha_0 = 1)$$

are of interest in the numerical solution of ordinary differential equations of first order. Given the coefficients α_λ with $\Sigma\alpha_\lambda = 0$, the requirement $Lx = 0$ for all polynomials $x(t)$ of appropriate degree determines uniquely the coefficients β_λ and leads to classical integration formulas such as Adams' formula. Their trigonometric counterparts turn out to have coefficients β_λ which depend on the parameter $v = 2\pi h/T$, and methods of (trigonometric) order p exist whenever $|v| < \min\,[v_p, 2\pi/(2p - 1)]$, where v_p are zeros of certain well-defined trigonometric polynomials.

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[1] *Math. Panel Ann. Progr. Rept. Dec. 31, 1959*, ORNL-2915, p 1; *Dec. 31, 1960*, ORNL-3082, p 1.

[2] Walter Gautschi, "Numerical Integration of Ordinary Differential Equations Based on Trigonometric Polynomials," *Numerische Math.* **3**, 381–97 (1961).

Functionals

$$Lx = \sum_{\lambda=0}^{k} \left\{\alpha_\lambda x[(k-\lambda)h] - h^2\beta_\lambda x''[(k-\lambda)h]\right\} \qquad (\alpha_0 = 1)\,,$$

useful for second-order differential equations, have also been studied from this point of view. Trigonometric counterparts of Störmer's extrapolation and interpolation formulas have been derived and tested on differential equations $x'' + P(t)x = 0$ with slowly varying positive $P(t)$. Notable gains in accuracy were observed.

GAUSSIAN QUADRATURE FORMULAS FOR SPECIFIC WEIGHT FUNCTIONS

During the past two decades many efforts have gone into the calculation of tables pertaining to Gaussian quadrature formulas for various specific weight functions. Work is in progress to develop a machine program which would produce zeros and Christoffel numbers relative to any weight function $w(x)$ for which the moments $m_k = \int x^k\, w(x)\, dx$ can be calculated. Such a program has already been written and tested for classical weight functions and some others, notably $w = \ln(1/x)$ for $0 < x \leqq 1$, and $w = E_n(x)$ (the exponential integrals) for $0 < x < \infty$. Existing tables[3,4] pertaining to the last two weight functions have been extended.

Presently, Gaussian quadrature formulas are being constructed relative to the weight function

$$w(x) = \frac{1}{2x}\,\frac{1}{(A + \frac{1}{2}\ln x)^2 + (\frac{1}{2}\pi)^2} \qquad (0 < x \leqq 1)\,,$$

where A is constant. This function arose as a result of efforts to evaluate some rather complicated integrals occurring in a study of neutron transport theory.[5] The function has a logarithmic singularity at $x = 0$, where it behaves like $x^{-1}\ln^{-2} x$, but numerical experiments indicated that the use of $x^{-1}\ln^{-2} x$ as weight function in $[0, e^{-1}]$ does not yield the desired accuracy for larger values of A. The moments of $w(x)$ are

$$m_0 = 1 + \frac{2}{\pi}\tan^{-1}\frac{2A}{\pi}\,,$$

$$m_k = -\frac{2}{\pi}\, Im\left[e^{-2kA+ik\pi}E_1(-2kA + ik\pi)\right] \qquad (k > 0)\,,$$

where E_1 denotes the exponential integral $E_1(z) = \int_z^\infty (e^{-t}/t)\, dt$.

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[3]H. Mineur, pp 555–56 in *Techniques de Calcul Numérique*, Paris, 1952.

[4]A. Reiz, "Quadrature Formulae for the Numerical Calculation of Mean Intensities and Fluxes in a Stellar Atmosphere," *Arkiv Astron.* 1(13), 147–53 (1950).

[5]W. Kofink, *Studies of the Spherical Harmonics Method in Neutron Transport Theory*, ORNL-2901, p 5 (February 1960).

A posteriori estimates can be given for the accuracy of zeros and Christoffel numbers by computing the moments with the help of the constructed quadrature formula and comparing the results with the input values for the moments. The observed deviations can be shown in a first approximation to be linearly related to the errors of the zeros and the Christoffel numbers. The relative matrix (apart from a diagonal matrix factor containing the Christoffel numbers) is a confluent Vandermonde matrix in the zeros x_ν,

$$U_{2n} = \begin{pmatrix} 1 & 1 & \dots & 1 & 0 & 0 & \dots & 0 \\ x_1 & x_2 & \dots & x_n & 1 & 1 & \dots & 1 \\ x_1^2 & x_2^2 & \dots & x_n^2 & 2x_1 & 2x_2 & \dots & 2x_n \\ \vdots & & & & & & & \vdots \\ x_1^{2n-1} & x_2^{2n-1} & \dots & x_n^{2n-1} & (2n-1)x_1^{2n-2} & (2n-1)x_2^{2n-2} & \dots & (2n-1)x_n^{2n-2} \end{pmatrix}.$$

The error estimates alluded to can be expressed in terms of norm estimates for the inverse of U_{2n}. Adopting the matrix norm $||A|| = \max\limits_{1 \leqq \nu \leqq n} \sum\limits_{\mu=1}^{n} |a_{\nu\mu}|$, one shows[6] that

$$||U_{2n}^{-1}|| \leq \max_{1 \leqq \lambda \leqq n} b_\lambda \left(\prod_{\nu \neq \lambda} \frac{1 + |x_\nu|}{|x_\nu - x_\lambda|} \right)^2,$$

where

$$b_\lambda = \max \left[1 + |x_\lambda|,\ 1 + 2(1 + |x_\lambda|) \sum_{\nu \neq \lambda} \frac{1}{|x_\nu - x_\lambda|} \right].$$

MATRICES

Among the recently developed inclusion theorems for matrices,[7] one suggests a possible method for finding individual roots of the matrix. This theorem asserts, in part, that if A is a normalizable matrix, then associated with any vector $x \neq 0$ there is a family of inclusion disks (i.e., each known to contain at least one root), and that among these disks there is a smallest, which has its center at the Rayleigh quotient $x^H Ax/x^H x$. Any disk of the family may be called a Temple disk, and the least of those the Weinstein disk belonging to x. The disks seem to be the simplest useful inclusion regions.

It is natural to attempt to develop a sequence of vectors x_i such that the Weinstein disks belonging to them shrink to a point. This point will then be a characteristic root, and the vector to which it belongs will be the characteristic vector belonging to that root. And for this purpose it is natural to select a

[6] Walter Gautschi, "On Inverses of Vandermonde and Confluent Vandermonde Matrices," to be published in *Numerische Mathematik*.

[7] A. S. Householder (with F. L. Bauer), "Moments and Characteristic Roots," *Numerische Math.* 2, 42–53 (1960).

second vector y, perhaps $y = Ax$, linearly independent of x, and to find a vector in the plane of x and y whose Weinstein disk is smaller.

To find the vector with the smallest possible Weinstein disk requires the solution of an algebraic equation of degree three at least. Hence this is not feasible. But by solving a quadratic equation it is possible to find the vector whose concentric Temple disk is the smallest possible, and the Weinstein disk can be no larger. Thus a diminishing sequence of Weinstein disks can be obtained.

Some starting vectors x lead to Weinstein disks that shrink rapidly to points; others do not. Often the sequence of disks appears to converge to a limiting disk containing several roots. In such cases there seems to be no advantage in selecting y otherwise. Nevertheless, it would be highly desirable to have a procedure that leads from an arbitrary (or almost arbitrary) vector x to a sequence of vectors x_i that necessarily converges to some characteristic vector, and not always the dominant one as is the case with simple iteration.

A modification that looks hopeful and is now being investigated is to combine this method with the Rayleigh-quotient method. The Rayleigh-quotient method is defined by sequence $(A - \lambda_i I)x_{i+1} = x_i$, $\lambda_{i+1} = x_{i+1}^H Ax_{i+1}/x_{i+1}^H x_{i+1}$, starting with an arbitrary $x \neq 0$. This method is known to converge quite rapidly under rather general circumstances, but has the disadvantage of requiring the solution of a system of equations at each step. Thus more computations are required in a step of the Rayleigh-quotient method than in a step of the Weinstein-circle method. It is proposed to interpose a step of the Rayleigh-quotient method whenever the Weinstein-circle method appears to be slowing up.

Programming and Programming Research

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The activities of the Mathematics Panel in programming and programming research consisted to a considerable extent in the continuation, completion, and extension of activities already described in detail in the preceding progress report.[3] The status of the projects is briefly summarized, while additional projects are described more fully. For convenience the work is divided into five parts and is reported here accordingly: (1) programming research, (2) cooperative ALGOL efforts, (3) the Oracle ALGOL translator, (4) Oracle simulation studies, and (5) general-purpose programs other than systems programs.

PROGRAMMING RESEARCH

Development of ALGOL Translation Techniques

It was mentioned in a previous progress report[4] that specifications[5] for an ALGOL 60 translator which realize a simplification of the Bauer and Samelson translation techniques had been drawn up. These specifications are being revised to encompass more details. The revision will also include the treatment of dynamic declarations and a full analysis of procedures.

Handling of Procedures

The rather general discussion of this section represents a summary of the present approach to the problem of procedures. The development of details is in progress. Recursive procedures are not being considered.

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[1]Cooperating programmers from the Control Data Corporation.

[2]Neutron Physics Division.

[3]G. J. Atta *et al., Math. Panel Ann. Progr. Rept. Dec. 31, 1960,* ORNL-3082, p 5.

[4]*Ibid.,* p 22.

[5]A. A. Grau, *Structure of an Algol Translator,* ORNL-3054 (Jan. 23, 1961).

Each parameter of a procedure call will be converted into a subroutine. This will be done in such a way that procedure call and procedure declaration are translated independently of each other. The subroutines for each call will follow in natural order the transfer of control to the procedure body. For simple variables the subroutine need consist of only one word, provided that the procedure body contains coding which picks up the word and places it in a reserved location in the body. The procedure body also contains code to provide the linkage to this reserved location. Parameters other than simple variables generally require more than one machine word, and in these cases the work picked up by the procedure body contains reference to the subroutine for that parameter. In all cases the subroutine delivers an address.

This rather general linkage between procedure body and procedure call is made necessary by the ALGOL concept of "call by name." The work on procedures outlined in the last progress report[3] did not include the handling of call by name. Roughly, this means that the procedure body must be able to reach back to the appropriate procedure call each time a parameter is referenced. The simpler notion of "call by value" is handled by a variation of the above technique, but the variation must be in the body rather than in the call.

Storage Allocation

The storage-allocation problem has been solved. Since recursive procedures are not being considered, storage can be assigned to simple variables and information vectors at translation time. The mechanism is nontrivial, however, if one desires the economy made possible by the block structure of ALGOL 60. In particular, if procedure P is declared in block B, then the storage for simple variables and information vectors local to procedure P must not conflict with that assigned to those local to other procedures declared in B or blocks contained in B. On the other hand, blocks which cannot be activated at the same time during execution of the program may share storage.

The following is a description of the required mechanism. Four lists are required: (1) V, the variable push-down, (2) T, the block-tracing push-down, (3) R, the procedure maximum serial number push-down, and (4) S, a list of sentinels. It is convenient to make V a double-entry list. If we consider these lists as one-dimensional arrays with subscript values denoted by m, then the mechanism (for simple variables only) is determined by operations at five points:

1. when **begin** is encountered,
2. when **procedure** is encountered,
3. when each variable declared is encountered,
4. when the end of the declarations for a block is encountered, and
5. when **end** is encountered.

The mechanism associates a serial number $R[m]$ with each identifier. The serial number is then the symbolic or relative address.

The Dynamic Type-Handling Problem

A practical difficulty in implementing ALGOL arises from the fact that in mathematics (and therefore in ALGOL) the integers form a subset of the set of real numbers. On present computers, integers and real numbers are implemented by means of fixed-point and floating-point representations, respectively. These are usually disjoint sets. This feature imposes on ALGOL implementation either the necessity of handling types of variables dynamically, that is, information concerning the types of variables and intermediate results must be available at the time of execution of the target program, or some restrictions must be placed on the language used on a particular machine.

The possibility of avoiding this difficulty by using fixed-point and floating-point number representations of a slightly different kind from those currently used was investigated. This resulted in the design of a representation and normalization scheme which establishes a relationship between fixed-point and normalized floating-point numbers that corresponds to the historical relationship between integers and real numbers. The new system appears to have no disadvantages over the usual representations and can be implemented on machines either by suitable subroutines (where floating-point operation is attained this way) or by suitable hardware. The use of such a representation would avoid satisfactorily the use of duplicate machine operations for a given mathematical operation and would make possible considerable simplification in the translation of algorithmic languages such as ALGOL.

ALGOL Exposition

The ALCOR group, an association of institutions cooperating very closely on the construction of ALGOL translators and on a common hardware representation for their machines, provided a common manual[6] for their users. This manual was translated from German into English and revised to conform to ALGOL 60. It serves as an introduction to ALGOL and emphasizes the normal use of the basic subset of the language. It is expected to be used in ALGOL programming training and as an elementary exposition for a wide class of readers.

Another exposition[7] was written to describe in good detail the features that make ALGOL a powerful programming tool. It was intended for experienced programmers and gives a more thorough and sophisticated view of the language.

COOPERATIVE ALGOL PROJECTS

ALGOL Syntax Checker for SHARE

The syntax checker for the SHARE ALGOL compiler is based on the syntax of ALGOL as described in the ALGOL 60 report.[8] The program is designed to be very flexible with a processor for each type of

[6] R. Baumann (ed.), *ALGOL-Manual der ALCOR-Gruppe*, Johannes Gutenberg University, Mainz, March 1961.

[7] H. H. Bottenbruch, *Structure and Use of ALGOL 60*, ORNL-3148 (July 12, 1961).

[8] J. W. Backus *et al.*, "The Algorithimic Language ALGOL-60," *Communs. Assoc. Computing Machinery* 3, 299–314 (1960).

statement or expression. These processors are completely recursive; that is, any processor may call any other processor, including itself, to scan a particular set of symbols.

The flow of control from one processor to the next is supervised by a recursive entry subroutine which stores the calling location in a push-down list and transfers control to the requested processor. Return from a lower-level processor to the calling processor is controlled by a recursive return routine which takes the last entry point from the push-down list and uses it to set up the return. An auxiliary push-down list is used to store information needed for recursive calls of certain processors.

A processor consists of a set of tables of permissible symbols, each one of which has associated with it an "action location." When a match is found between the table symbol and the program symbol being scanned, control is transferred to the action location associated with the table entry. At this point the appropriate action is taken. For example, the symbol under scan may be put away for translation, the next symbol brought under scan, and then control is passed to the next segment of tables. If a permissible symbol match is not found during the scan of a table, an appropriate error message is written, and the checker enters the "resume" mode where it scans each expression as it encounters it, meanwhile watching for the beginning of a statement or block which will enable the processor to resume normal scanning. By use of the resume mode it has been possible to check most programs from beginning to end in spite of errors. It is true that this mode of scanning will sometimes produce false error messages where an actual error, for example, the omission of a semicolon between two assignment statements, will cause another apparent error to be noted where it does not really exist. However, it is felt that this is preferable to abandoning the program at the first error. A count is kept of all error messages as they are written, and if this number becomes too large the program is stopped with the suggestion that errors encountered to this point be corrected before further checking is done.

The Control Data Corporation 1604 ALGOL Processor

An implementation of the Algol translation specifications mentioned above is being investigated in a cooperative effort with the Control Data Corporation. Although the specifications are essentially machine independent, details are being worked out with the help of Control Data Corporation personnel for that company's 1604 computer. The above-mentioned IBM 7090 ALGOL syntax checker will be adapted to the 1604 and combined with the translator to create an ALGOL processor for the 1604. The processor will thus consist of two programs. A complete syntax check is performed before control is turned over to the translator. Plans call for two possible target codes, subject to programmer option. He may choose to use machine code produced in core storage, ready to run, or binary-coded-decimal (BCD) output on tape, ready as input to CODAP, the 1604 assembly program.

Mainly in the interests of target program efficiency, certain features of ALGOL 60 are not being handled. These restrictions are:

1. The Processor does not handle recursive procedures.
2. It does not accept **own** arrays having variable dimensions.

3. It imposes certain restrictions on the handling of type of variables. This is due to **real** quantities being handled in floating-point and **integer** quantities in fixed-point.
4. Quantities must be declared before they are used. Quantities not declared are treated as real simple variables.

Several of the basic subroutines have already been coded by Control Data Corporation personnel. Testing of these routines has begun and involves the translation of some simple assignment statements and arithmetic expressions. Much of the planning of the routines involved an attempt at maximum target program efficiency. For example, while it is simpler to store at once all intermediate results, this results in many instances in superfluous instructions in the target program. To avoid this, full use is made of the accumulator as temporary storage. The utilization of indirect addressing of array elements simplifies the target program but introduces some complication into the translation process.

ALGOL Maintenance

The Mathematics Panel continued its representation in the ALGOL Maintenance Group, a subcommittee of the Committee on Languages of the Association for Computing Machinery under the direction of J. H. Wegstein, Bureau of Standards, Washington, D.C. Originally there was strong feeling that revisions and changes in the language were desirable. The significant development of the year was an unofficial affirmative response to a memorandum prepared at Oak Ridge by F. L. Bauer, H. H. Bottenbruch, A. A. Grau, K. Samelson, and J. H. Wegstein. The memorandum favored the adoption of a resolution advocating no changes in the language at this time, the treatment of ambiguous features in the basic ALGOL report[8] as undefined (with no real loss of power in the language), and an emphasis on the construction of practical translators. A majority of the committee were in favor, though this was short of the 90% vote required for official action. Changes to the language, therefore, appear at this time unlikely, with the result that compiler implementors can proceed without fear that changes may invalidate previous work.

ORACLE ALGOL TRANSLATOR

Magnetic-Tape Files

Magnetic-tape files are used for data storage in the Oracle-ALGOL translator. This feature has been fully described.[9]

Implementation of magnetic-tape files has been completed. A program was constructed which scans all array declarations and builds up tables which for each array contain the information necessary for the translation process. The work done here parallels in many respects the work done previously for normal arrays only. Thus segment III of the translator underwent severe revisions in order to incorporate the tape array information in the tables.

[9] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960,* ORNL-3082, pp 14–15.

Both normal arrays and tape arrays are handled in a particularly simple way in the Oracle-ALGOL translator. Whenever an element of an array (subscripted variable) appears in a program, the translator activates a subroutine (called "address calculator") which computes the numerical address of that element and places it in a special location. Call this location *ADD*. This numerical address characterizes the array being used. For example, the addresses used for normal arrays range from 0 to $2^{11} - 1$, and those for tape arrays range from 2^{32} to $2^{35} - 1$.

In exit from the "address calculator" the translator inserts instructions to use the address of the subscripted variable in the case of normal arrays. For tape arrays, however, another subroutine (called "tape positioner") is called on exit from the "address calculator." On exit from the "tape positioner" the required tape location is represented in high-speed storage, and its associated high-speed storage address is in location *ADD*. This address can be used in the same way as an ordinary subscripted variable.

When supplied with a tape address in location *ADD*, the "tape positioner" controls the necessary tape motions and transmissions and replaces the tape address in *ADD* by a high-speed storage address.

The translation matrix in segment IV of the translator has been modified so that the "address calculator" computes the addresses of both normal arrays and tape arrays, and instructions for calling the "tape positioner" have been inserted after the address of an element of a tape array has been computed. The processing of the symbol **stop** was modified to allow the programmer automatically to write on the appropriate magnetic tapes any information represented in high-speed storage. This feature is needed only when the write or read-write state is used. If tape files are used, the translator sets an entry into a subroutine that investigates the state of each magnetic tape and writes any information that needs to be on magnetic tape. This subroutine entry is followed by a stop order. If the Oracle ALGOL program does not use tape files, then the translator sets a stop order.

Multisegment ALGOL Programs

A program which is too long to fit into the full 2048-word memory of the Oracle must be divided into segments.

Two new delimiters have been added to the language. Strings of one or more statements may be combined into a segment by enclosing them within the "segment parentheses" **segment begin** and **segment end.**

To make automatic switching of segments in ALGOL multisegment programs, two new statements have been introduced into the language:

1. **Advance** n **segments.**
2. **Recede** n **segments.**

The first statement causes the Oracle to skip the next n segments in sequence, to place the one immediately after that into high-speed memory, and to transfer control to the beginning of that segment. The second statement causes the Oracle to skip the segments in sequence preceding the current one, to place the one immediately preceding these into high-speed memory, and to transfer control to the beginning of that segment.

The major task here was the construction of a subroutine to implement the above specifications.

The *for* Statement

The ALGOL 60 **for** statement was fully implemented in Oracle ALGOL. A complete description of the method is found in the previous progress report.[9] In order to implement this **for** statement, segment II was completely recoded. Moreover, segments III and IV had to be revised to take into account several auxiliary statements used to preprocess the **for** statement.

Other Work on the Translator

Segments III and IV underwent some other revisions which brought Oracle ALGOL in closer conformity with ALGOL 60.

The array declaration in use in the Oracle ALGOL has the form of the array declaration of ALGOL 58. Segments I and III were revised to accept the form of the array declaration of ALGOL 60. This entailed recoding those parts which constructed the array tables. However, it involved no changes on segment IV.

The down arrow ↓ which was used in ALGOL 58 as the right-hand parenthesis of exponentiation,

$$a^b = a \uparrow b \downarrow ,$$

was eliminated. Segment IV now follows the rules of ALGOL 60 by which

$$a^b = a \uparrow b .$$

Although the Oracle ALGOL translator processed codes involving the option (**if** ... **then** ...) and the alternative (**if** ... **then** ... **else** ...) in agreement with ALGOL 60, internally the symbol **then** was changed in segment I to semicolon ";". This did not create a serious inconvenience and shortened the translation matrix slightly. However, in preprocessing the ALGOL 60 **for** statement, the symbol **then** is also introduced. In this connection it may not be treated like a semicolon. Hence the translation matrix was extended to accept the symbol **then.** Incidentally, this eliminates the possibility of syntactical errors of the form **if** B ; S (where B stands for a Boolean expression and S for a statement).

Another modification of segment IV makes the minus sign "–" agree with ALGOL 60 as far as arithmetic expressions are concerned. In line with this the **punch** order was revised to accept the statement

$$\textbf{punch} - E$$

(where E stands for an expression whose first symbol is not minus). This was improperly translated.

Moreover, the length of the label tables, the unsatisfied address table, and the push-down lists were altered to make better use of the high-speed storage. Practical experience made obvious the need for these changes.

Switches were studied, and a tentative plan was considered to process switch declarations and statements of the form

$$\textbf{go to } s[i]$$

where s is a switch. This work was discontinued.

Finally, some features needed to allow a restricted version of procedures (ref 10) in Oracle ALGOL were incorporated. However, further work on procedures for this translator has been discontinued.

ORACLE SIMULATION STUDIES

As no computer has been or will be useful indefinitely, simulation of the Oracle on some other digital computer was studied. The Oracle was specially built, and no other computer can correctly execute Oracle programs. The usefulness of many programs outlive the usefulness of the computer, and reprogramming is expensive. Programs which are not used enough to economically justify reprogramming but which would have to be replaced can be grouped together to justify the expense of programming a simulator.

In considering the logical design of the Oracle and the execution time under simulation, it was decided that the simulator would be written for a high-speed digital computer with word length of at least 41 bits, no less than 12,000 words of high-speed storage, paper and magnetic tape input/output, on-line typewriter, complementary arithmetic, and index registers. With enough core storage available, the main consideration is speed of execution under simulation.

Representation of Oracle Word

For all Oracle instructions, except some transfers, there is a need to refer to Oracle storage; therefore an exact duplication of Oracle storage appears in the simulator.

Simulation computer	$\beta_0, \beta_1, \beta_2, \dots \beta_{39}, \beta_{40}$
Oracle	$\beta_0, \beta_0, \beta_1, \dots \beta_{38}, \beta_{39}$

If the simulation computer has more than 41 bits, the rightmost unused bits of the simulation computer will be zero so as not to contribute to arithmetic operations. If the Oracle word were right-adjusted, either the sign bit would have to be duplicated in the extra bits at the left, or every Oracle instruction in which the sign bit must be determined would take longer to execute (e.g., add magnitude, conditional transfer). If the sign bit is duplicated, the duplication must be renewed after every Oracle instruction which could change the sign. Therefore the preferable choice is to left-adjust the Oracle word, with the sign bit duplicated once. This corresponds to the Oracle hardware where the sign bit of an operand is actually duplicated for transmission to the forty-first stage of the adder. Thus the sign bit should be duplicated for all words in Oracle memory and for the interpretive Oracle Q register. This enables the leftmost bit of the interpretive accumulator to become the so-called A_x bit. With the above configuration, overflow can easily be determined by comparing the leftmost two bits in the interpretative accumulator.

[10] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, pp 16–19.

Execution of Oracle Instructions

Inasmuch as each Oracle instruction is independent of the one preceding it, it was decided to have a closed instruction subroutine for every defined Oracle instruction, with the exception of curve-plotter instructions. As the simulation computer need not have a curve plotter, curve-plotter instructions will be treated as undefined instructions. All undefined instructions will cause simulation to stop with a message on the on-line typewriter or to be executed as no operation, at the Oracle programmer's discretion.

At first, Oracle instructions were to be decoded into the instruction subroutine entry and Oracle execution address each time an Oracle instruction was to be executed.

It was later found that simulation time could be considerably reduced if the instruction subroutine entry and Oracle execution address were saved. This causes the simulator to become, in part, a translator.

To effect this partial translation, two tables in addition to the one containing an exact duplication of Oracle memory, ORACLE, and a decoding subroutine are required. The first is an executable table, CONTROL, which has two instructions, a load-index register with the contents of its address followed by a transfer to some location, for every Oracle instruction. A designated index register simulates the Oracle control counter. It contains the location in CONTROL corresponding to the Oracle instruction to be executed next. The last two instructions in CONTROL put the address of CONTROL corresponding to the right instruction of Oracle *000* in the simulated control counter and transfers to the location in CONTROL corresponding to the left instruction of Oracle *000*. This allows simulation of following the right instruction of Oracle *7FF* with the left one at *000*.

The other table, ITT, contains two instructions for every possible Oracle instruction. The first instruction is a test on some external sense switch which simulates the breakpoint switch. If the switch is set, transfer is made to a breakpoint routine which outputs the breakpoint stop and stops simulation. If the switch is not set, the second instruction, a transfer to an instruction subroutine, is executed. The table is designed such that if an Oracle instruction is considered as a number its corresponding subroutine entry may be found easily.

When an Oracle problem is loaded, all transfers from CONTROL are to the decoding subroutine. To execute the Oracle program, the simulation control counter is set and a transfer is made to the location in CONTROL corresponding to the location in Oracle to be executed. The decoding routine finds the Oracle instruction in ORACLE, places the execution address of the Oracle word to be executed in the address of the first of the two corresponding instructions in CONTROL, and places the proper instruction subroutine entry found from ITT in the second. If the Oracle address has the breakpoint bit, the address of ITT that contains the breakpoint switch test preceding the proper subroutine entry is placed in the address of the second of the two corresponding words in CONTROL instead of in the proper instruction subroutine entry. The decoding subroutine also enables the right-hand portion of the Oracle word to be preserved for the next execution only, if the left instruction in that same Oracle word would store some information into the right-hand portion of that word. The decoding subroutine exits to the instruction preceding the one which transferred into it.

Instruction subroutines increase the simulation control counter or change it completely, as necessary.

Once an Oracle instruction and execution address have been decoded, no further reference is made to ORACLE when that instruction is to be executed, unless that work in ORACLE is changed by some Oracle instruction. The instruction subroutine which changes the word in ORACLE also places the address of the decoding subroutine entry into the corresponding location of CONTROL, causing a transfer to the decoding subroutine the next time that Oracle instruction is to be executed. Every time a word of Oracle is to be used as an operand, it is taken from ORACLE.

Console Simulation

An on-line typewriter for the simulation computer is necessary for three reasons. The most obvious is to simulate the Oracle console typewriter. Next, it can print messages from the simulator. Most important, it can be used to simulate the complete Oracle console. All instructions given from the Oracle console keyboard and the setting of the no-write switches will be given from the typewriter.

The typewriter will also print error messages for many of the error lights on the Oracle console.

This means that not only does CONSOLE, the routine which controls simulation of the Oracle console, have to be able to use all the instruction subroutines but that all the paper and magnetic tape instructions must be able to use CONSOLE.

Magnetic Tape

All available high-speed digital computers on which the Oracle can be simulated have magnetic tape units which are similar in two respects: (1) once information has been written on the tape no information following it which was previously written can be read, and (2) the tapes can be read or written in the forward direction only. Oracle tapes have neither of these restrictions. Being able to read or write only in the forward direction presents little problems in simulation, because the order of information may be reversed after reading or before writing. The first restriction is more serious.

It will take at least three tape units and much computer time to simulate each Oracle wide-magnetic-tape unit if no way can be found to write on magnetic tape and still be able to read following information that was previously written on it. Inability to read previously written information seems to be due to tape slippage. To try to keep this slippage from disturbing the information following a record, blank tape is being written after each record. Experiments have not been completed, but at present the method seems to work at least with IBM 729 IV and with Ampex tape units. If records may be rewritten reliably 30 times without disturbing other information on the tape, the method will be accepted. It is realized that no matter what method is used, the tapes which simulate the Oracle wide magnetic tapes will have to be rewritten often.

If the simulation computer has more than 12,000 words of high-speed core storage, the rest of the core will be used to simulate the wide magnetic tape. This would allow buffering-in of information before it is needed and hopefully would prevent the reading of a block of data more than once from tape.

GENERAL-PURPOSE PROGRAMS

Response Surface Analysis

The Linear Regression Program was completed this past year and will provide a complete response surface analysis, except for the eigenvalues and eigenvectors which determine the shape of the response, the transformation relationship between the axes of the response, and the axes of the experimental design. It did not seem economical to include the latter in the final program, since the computation can be readily carried out as a separate problem, using the eigenvalue and eigenvector codes.

In addition to the usual regression analysis, it is now possible to obtain an analysis-of-variance table and a table for an analysis-of-variance regression model, which is a breakdown of the treatment sums of squares.

If the regression equation is quadratic, the optimum point or stationary point value can be computed from the system of linear equations,

$$\frac{1}{2}\frac{\partial y}{\partial x_s} = 0, \qquad s = 1, 2, \ldots, k .$$

The solution vector $x^0 = (x_1^0, x_2^0, \ldots, x_s^0)$ gives an estimate of the optimum level of each factor.

This code is available as a canned program.

Gaussian Integration Routines

Routines for single, double, and triple integration have been written in FAP and made compatible with the ORGDP 7090 monitor system and its error-trace routine. These routines, GINT1, GINT2, GINT3, which follow closely a similar set of IBM 704 routines written by Marjorie P. Lietzke, can be used with FORTRAN programs and subroutines as well as with FAP codes. Details on the use of these programs are given in a report.[11]

[11] M. B. Emmett *et al.*, *IBM 7090 Gaussian Integration Routines*, ORNL CF-61-5-54 (Dec. 6, 1961).

Biology and Medicine

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D. G. Gosslee J. E. Parham

The services rendered by the Biometrics Section during the past year covered a broad area of applications in cytology and genetics, pathology and physiology, radiation immunology, mammalian recovery, microbial protection and recovery, mammalian genetics and development, and cell physiology. The basic problems in these areas involved construction and testing of mathematical models describing biological systems, estimation of mortality intensities, fitting multitarget survival curves, and bioassay analysis. In addition, the usual statistical techniques, such as the analysis of variance, regression analysis, confidence-limit estimation, and hypothesis testing, were applied to numerous problems in biology.

The establishment and final approval of a biomedical-data recording unit has been an important contributor to the increased use of high-speed computers. The availability of IBM electronic accounting machinery has automated much of the data recording for the Biology Division. As a direct consequence, increased use was made of the electronic data-processing equipment at the Y-12 Plant and ORGDP in all areas of numerical investigation.

Considerable emphasis was placed on problems in nonlinear estimation. The iterative least-squares procedures which may be employed in attacking such problems are indeed time-consuming when handled by small computers. On the other hand, experience gained from the use of the IBM 7090 earlier this year indicated that a large assortment of such problems could be handled very rapidly and very successfully by a high-speed computer. Several new and complicated nonlinear biological models, for which subroutines were written, have been tested with existing experimental data. The degree of success in this area of endeavor has been satisfying. However, increased use of the computers will be necessary to enable closer investigation of the problems for which the models failed partially or completely.

Finally, a program was written in FORTRAN language for the IBM 7090 for the analysis of variance for data in two-way classifications when the numbers of observations in each cell are unequal. Any combination of six standard methods can be used to analyze one or more sets of data. In five of the methods a set of weights is calculated for the method chosen and then a weighted analysis of variance is computed. The sixth method, fitting constants, uses an iterative procedure that converges to the exact least-squares solution. The program was prepared for the analysis of ORNL data and for an empirical comparison of the six methods.

BIOMEDICAL-DATA RECORDING

The collection and recording on IBM cards of biological experimental data was intensified during this report period. These data were prepared on IBM machines in the Biology Division and processed on computers at ORNL, the Y-12 Plant, and ORGDP.

IBM machines received on a rental basis during this year were one 083 sorter, one 085 collator, and one 519 document-originating machine. At present the recording unit has these machines as well as one 026 card punch and one 056 card verifier. At the end of the year, machine utilization amounted to approximately 200 hr/month.

Data from the Mammalian Genetics and Development Section and the Pathology and Physiology Section continued at about the same volume as last year. Calculation and tabulation of these data were done at Y-12 on an IBM 1401 data processing system which was installed at midyear.

Experimental data from the following sections of the Biology Division were put on a punched-card system:

1. Cytology and Genetics
   (*a*) Paramecium mutation. Data are punched on a routine basis. These cards, about 200 per week, are processed on the IBM 7090 system at ORGDP.
   (*b*) Neurospora. Work sheets containing data were received from this section late in December. The information from these experiments is being punched on cards.
   (*c*) Drosophila. A small amount of information has been accumulated pertaining to these experiments.
2. Radiation Microbiology. A small number of cards have been punched from information received from the Bacterial Genetics Group.
3. Mammalian Recovery. Work sheets from the Hematopoietic Recovery Group's bone-marrow studies were received late in the year. Approximately 800 cards/week are being punched.

Preliminary conferences have been held with individuals in the following groups for the purpose of recording data on punched cards:

1. Biology Division
   (*a*) Pathology and Physiology (Long-Range Study)
   (*b*) Cell Physiology
   (*c*) Chemical Protection and Enzyme Catalysis
   (*d*) Experimental Animal Facility
2. Health Physics Division
3. ORINS Biomedical Division

The following programs have been written for use on the IBM 1401:

1. Specific locus mutation intervals and tabulation
2. Specific locus mutation listing
3. Calculation of animal autopsy records
4. Tabulation of animal autopsy records
5. Summary tabulations for animal autopsy records
6. Calculation and punching of drosophila counts

CYTOLOGY AND GENETICS

The theory concerning induction of two-break chromosome exchanges by sparsely ionizing radiation would imply that exchanges increase as the 1.5 power of the dose. In explaining this phenomenon it is assumed that exchanges are two-hit events which should increase as the square of the dose $(Y = kD)^2$ and that the discrepancy is caused by the relatively large numbers of inviable exchanges at high doses in *Drosophila* and by the production of one-hit as well as two-hit exchanges in *Tradescantia*. This explanation, which amounts to an interposition of extraneous factors to account for the shape of the response curves, would indicate that some imperfection exists in the underlying mathematical model. Consequently a study was carried out to find a mathematical model based on the biological phenomena, which are assumed to be interacting, and to test this model with data collected in the laboratories.

It was assumed that there are only a limited number of sites in a cell where chromosomes come close enough to rejoin and form an exchange if broken. Since breaks are distributed at random and are proportional to the dose of irradiation, the probability of not breaking a chromosome in one of these sites is given by $e^{-k_1 D}$, where D is the dose. Thus the probability of at least one break in a chromosome is $1 - e^{-k_1 D}$, and the probability of at least one break in each of two chromosomes is $\left(1 - e^{-k_1 D}\right)^2$. (The necessity of breaking two chromosomes at a site is a requirement for the formation of an exchange.) If a cell has n effective sites, then the expected yield per cell is given by $Y = n\left(1 - e^{-k_1 D}\right)^2$. Laboratory data for this model were fitted by nonlinear least-squares methods with excellent results. However, one observation made after fitting this model was that at low intensities the curve changes shape from one that increases more rapidly than the first power of dose and approaches a linear form. One explanation of this is that the linear component at very low intensities might be the result of the densely ionizing "tails" seen on the electron tracks produced by gamma and x radiation. To account for this linear component it was reasoned that the probability of not getting two broken chromosomes by a two-hit mechanism is $1 - \left(1 - e^{-k_1 D}\right)^2$, and the probability of not getting two broken chromosomes by a one-hit mechanism is $e^{-k_2 D}$, where k_2 is the average number of sets of two individual chromosomes broken by a single particle per rad per site. Thus the probability of the joint event is $e^{-k_2 D}\left[1 - \left(1 - e^{-k_1 D}\right)^2\right]$, and the probability of its nonoccurrence is $1 - e^{-k_2 D}\left[1 - \left(1 - e^{-k_1 D}\right)^2\right]$. The expected yield, therefore, per cell with n sites is given by

$$Y = n\left\{1 - e^{-k_2 D}\left[1 - \left(1 - e^{-k_1 D}\right)^2\right]\right\} .$$

Laboratory data for this more comprehensive model were fitted by nonlinear least-squares methods.

Successful use of high-speed computer programs for these fits has been dependent upon the extent of the available data and the reliability of the initial estimates of the parameters. That the model adequately represents the biological situation is not doubted. However, further study of the existing computer programs is necessary to determine better criteria for convergence of the iterative process.

One interesting by-product of the final model appears when it is expanded in power series, eliminating powers of D higher than 2. The result is of the form $Y = \alpha D + \beta D^2$, a quadratic expression suggested in biological literature as a model for the yield of chromosome exchanges per cell.

The production of aborted ascospores from crosses of *ad*-3 mutants with a cytologically normal wild-type strain can be used as a screening method to estimate the frequency of this class of genetic alteration among *ad-3* mutants of different mutagenic origins. In two random samples of ejected ascospores from 158 *ad-3* × wild-type crosses of *Neurospora crassa*, the frequency of aborted ascospores was determined and compared with a control cross of wild-type × wild-type. The proportion of *ad-3* mutants which produced a greater-than-control frequency of aborted ascospores varied as a function of mutagenic origin. As spore abortion patterns are known to occur in crosses of *Neurospora* strains carrying a gross chromosomal rearrangement, these results indicate a difference in the kind of genetic alteration induced by the various mutagenic agents. Chi-square tests for homogeneity were employed in the analysis of these data.

Mutation processes in paramecia subjected to various doses of irradiation and different chemical mutagens have been studied on a continuing basis. The data from such experiments are received for analysis on a weekly basis. These data are punched onto IBM cards and sent to the ORGDP Data Processing Center for analysis on the 7090 computer. The computer has been programmed to convert the data by a variance-stabilizing transformation, to analyze these transformed values, and to tabulate the results of the analyses in a form which is of immediate assistance to the investigator in setting up new experiments for the succeeding week. The whole operation, including punching, shipping, analysis, printing, and returning the data, is accomplished in 24 hr.

The incorporation of tritium-labeled amino acids into the nuclei of *Vicia faba* was analyzed by use of autoradiographs of isolated nuclei. Grain counts were made from 200 nuclei from each experiment, and the mean number of grains per nucleus for each experiment was determined. Plots of these data indicate that nuclear incorporation of basic amino acids is rapid and is found to some extent in all nuclei. The degree of labeling, however, begins to decrease immediately upon the addition of nonradioactive amino acids to the growth medium.

Sex-linked recessive lethals in *Drosophila* may be divided into two categories on the basis of their interaction with the Y chromosome. The first group are inviable in the presence or absence of the Y chromosome, whereas the second group survive in the presence of the Y but not in its absence. The first group are termed orthodox lethals and represent a mixture of chromosome-rearrangement-associated lethals and point-mutation lethals. The second group are termed Y-suppressed lethals and have been shown to be almost exclusively associated with chromosome rearrangements. The kinetics of induction of the two types of lethals should consequently be different, and an understanding of the dose-effect relations of the Y-suppressed should supply some insight into one of the components of the orthodox-lethal results. Several mathematical models have been fitted to existing data in an effort to estimate the parameters which explain the kinetics of lethality. The models, which are nonlinear, have been fitted by least-squares procedures by use of the IBM 7090 computer. To date only partial success has been achieved. The problem is being studied further.

MAMMALIAN GENETICS AND DEVELOPMENT

Data on skeletal abnormalities in offspring of irradiated mice collected in several experiments were examined to determine whether frequencies of abnormalities occurring only once (class 1) in an experiment and those occurring more than once (class 2) per experiment were different from the frequencies observed in the controls. The numbers were arrayed in 2 × 2 contingency tables so that the hypothesis of homogeneity could be tested by the Fisher exact test. The results of these tests indicated that the proportion of class 2 abnormalities in irradiated groups does not differ significantly from that in controls. Class 1 abnormalities, however, were significantly higher in irradiated groups than in controls.

During the past year all the data from the specific-locus mutation experiments were punched onto IBM cards. Preliminary analysis of these data involved the tabulation of frequency distributions of (1) sex ratio and (2) numbers of mutations by interval between irradiation of the sire and birth of the litter and by age of sire at time of irradiation, and (3) the size of litter by age of sire at time of irradiation. The frequency distributions were determined and tabulated by use of the IBM 1401 computer. At present these data are being studied for possible correlations of functional relationships between the time intervals and sex ratio, mutation rates, and litter size. One of the problems encountered in such a study is to find an appropriate technique for pooling data from several experiments. Thus, for example, one wonders what the best weighting procedure would be for combining the data on mutations in several time periods for three experiments at 300-, 600-, and 1000-r levels of irradiation. One difficulty immediately apparent is that the induced mutation rate estimated in the 1000-r experiment is lower than that in the 600-r experiment (an odd phenomenon not yet fully explained). In any case, one cannot give more weight to the 1000-r experiment on the basis of higher dose. Alternative methods of weighting are being studied.

Cytological studies of irradiated mouse testes have been extended to doses and rates other than those previously reported. Counts of type A spermatogonia were made in testis sections from mice for combinations of doses and rates used, and Sertoli counts were made at the higher doses. A bias in counts of type A cells at high doses due to shrinkage of the testis was corrected by ratios to Sertoli cells. Effects of dose and rate were estimated by making statistical tests among the counts and the corrected counts for each combination.

MAMMALIAN RECOVERY

Experiments involving ultraviolet killing of mammalian cells have been performed as a direct outgrowth of the work done previously on x-ray killing. As the absorption of ultraviolet light might be expected to produce killing in much the same manner as absorption of equivalent quanta of energy in the ionizing wavelengths, an action spectrum was run by determining the survival curves for energies at various wavelengths known to be differentially absorbed by various cell components, such as nucleic acids and proteins. Analysis of the data is required both in order to determine the most probable shapes of the survival curves and to allow correction of the action spectrum for the variation in total absorption by cells exposed to energy at various wavelengths. Data from such experiments involving various quanta of ultraviolet light have been fitted to several mathematical models by nonlinear least-squares techniques. In general, the program written for the IBM 7090 has produced reasonable results in the sense of convergence to maximum-likelihood estimates. However, where the techniques have failed or where the parameters are estimated with a high degree of variability, no reason for such failure is apparent. Further studies of all the mathematical models are in progress, and we hope to be able to report more fully on these studies.

Data on survival at 30 days of mice exposed to radiation and then injected with bone-marrow cells which had been irradiated at different doses were analyzed. A graphical method of obtaining survival curves was checked by the fit obtained by the method of least squares. Two transformations of the data used prior to the calculations according to least squares were also compared. The graphical method gives very close agreement with the least-squares method, and the two transformations agree closely when the number of mice at each response point is the same and when the mean response is close to 50% survival. However, when the number of mice at each point is not nearly the same or when the mean response is not close to 50%, the graphical method is not a good approximation to the exact method, and the two transformations do not agree. The appropriate transformation can sometimes be chosen by considering the assumptions required in using each transformation.

RADIATION IMMUNOLOGY

When antibody-forming activity of spleen cells is assayed on a given day after an antigenic stimulus, the $\log_2$ relationship between antibody titer and viable-cell number is linear up to a certain cell dose, and the slopes of these regression lines are not significantly different, regardless of whether the response is primary or secondary. In addition, the slopes remain unaltered even after sublethal x-ray treatments. Furthermore, the magnitude of decrease in the primary and secondary antibody-forming activities of spleen cells after a given dose of x rays is approximately the same. Thus the apparent difference in radiosensitivity between primary and secondary responses among intact animals exposed to sublethal doses of total-body x irradiation is mainly due to the total number of competent cells surviving after radiation treatment. It follows then that radiosensitivity of secondary antibody-forming capacity of intact animals can be best shown with those given a minimum preimmunizing treatment, and radioresistance shown with those given a maximum preimmunizing treatment. The data from these experiments were compiled and plotted in the form of an inactivation curve in order to estimate conveniently the relative loss in antibody-forming activity of spleen cells after varying doses of x irradiation. The model proposed and fitted was a "multitarget" model given by the equation $Y_i = 1 - \left(1 - e^{-kx_i}\right)^n$, where x_i is the dose of x ray, Y_i the corresponding relative antibody-forming activity, k the sensitivity per unit dose, and n the "extrapolated target number." The parameters k and n were estimated by nonlinear least-squares techniques.

By similar use of regression techniques it has been demonstrated that the relative antibody-forming capacity of spleen cells of donor mice varies with age from 1 week to 29 months. A very rapid increase in activity is noted during the first month of age, with a less rapid increase between 1 and 8 months. The maximum antibody-forming capacity was achieved at approximately 8 months of age, with a gradual decrease over the subsequent 21 months of life.

In intact animals the mechanism of homograft rejection has been observed to be less radiosensitive than that responsible for titratable antibody formation, though the radiosensitivity of the former varies with the relative strength of the antigen involved. This phenomenon may be explained either by the action of distinct types of somatic cells or by the action of one cell type in both mechanisms with different numbers of potentially competent cells in each. To test these possibilities, isolated cells were used as active material, and the percentage decrease of activity following x irradiation for each type of reaction was compared. Heavily irradiated F_1 hybrid mice were used as in vivo test tubes, in which the homograft-rejecting activity of P_1 (1st parent) cells against P_2 (2nd parent) cells was evaluated by measuring the decrease of agglutinin formation by the latter cells. The inhibition of the P_2 cells was found to be a function of the P_1 cells present. Data expressed as a decrease from controls in $\log_2$ titer were found to decrease linearly with an increase in $\log_2 P_1$ cells.

With this evidence of a functional relationship between decrease in titer and numbers of P_1 cells, two sets of experiments were performed to determine radiation inactivation of homograft-rejecting capacity at the cellular level. The experiments were performed on C3H mice preimmunized against BL transplantation antigens, C3H mice preimmunized against rat RBC (red blood cells), and BL mice preimmunized against rat RBC, all exposed in vitro to varying doses of x irradiation. For each group the fractions of functional cells were plotted against x-ray dose. The results of these nonlinear least-squares fits indicated a significant difference in radiosensitivity between homograft reactivity and agglutinin synthesis of cells from the same C3H strain.

PATHOLOGY AND PHYSIOLOGY

The sample sizes necessary in the proposed long-term, low-level irradiation study were re-evaluated in light of additional information accumulated in more recent experiments. No changes have been proposed on the basis of this re-evaluation. The total sample size for each sex, strain, and radiation intensity will be 27,000 mice, with 10,000 mice each in controls and 5-r groups, and 1000 mice each at the 25-, 50-, 75-, 100-, 150-, 200-, and 400-r points. The sample sizes were determined so that the coefficient of the quadratic term in the equation $y = a + bx^2$ (where y is percent myeloid leukemia and x is dose of irradiation) could be estimated with an error of about 4%. The only contemplated reduction in sample size might be at the 200- and 400-r points. At these high doses the quadratic model no longer describes the response, and therefore smaller sample sizes may be envisioned. However, even in the presence of such a reduction in numbers at the 200- and 400-r points, the total sample size per experiment would not fall much below 26,000 mice. Another aspect of the long-range study to which much thought has been devoted is the question of serial sacrifice. It is of interest to know more precisely the latent period of a disease such as myeloid leukemia. At present the age of an animal at irradiation and the age at death are easily recorded. However, the investigator would like to have a better picture of the time of onset of a disease after irradiation. To produce this it is necessary to sacrifice animals at various times after irradiation so that autopsies may be performed prior to the actual time of death from a specific disease. Sample-size determination for such serial-sacrifice studies depends greatly on the incidence of the various diseases under study as well as on the mortality intensity from various diseases. To estimate sample size for such an experiment, it is necessary to determine how many animals are required at time 0 in order to guarantee that x animals are available for sacrifice at time t. Several preliminary estimates of sample sizes have been made for the serial-sacrifice studies. The logistic problems involved in raising the large numbers of mice required for all aspects of the long-range study have been discussed with members of the Pathology and Physiology Section. These discussions, involving data recording and retrieval, have resulted in a preliminary IBM card layout which includes information for each mouse in such a way that every individual may be identified with respect to its place in the experiment as well as its lineage from the progenitors of the colony under study.

Estimates of numbers of mice needed in an experiment to study the occurrence of myeloid leukemia in mice exposed to fast neutrons were made. Five groups exposed at different levels and a control group will be studied for incidence of myeloid leukemia as well as other end points. The numbers of mice required in each group in order to have an 85% chance of detecting a given difference in incidence from group to group was estimated.

The effects of radiation on aging in mice were studied by measuring the temperature at maximum tension in a muscle fiber taken from the tail when this fiber is suspended in a water bath and the temperature of the water is raised. The linear regression of temperature on age was typified by large deviations of individual fibers from the regression. It was not possible to balance the selection of fibers of different length and thickness with selection of sex of mice. These factors and a change in tension through time are being investigated.

A statistical design was developed for an experiment in which mice that had been given a lethal dose of radiation (950 r) were given protective transplants of hematopoietic cells. The hematopoietic cells were exposed to seven radiation doses from 0 to 600 r and injected in varying amounts to obtain survival responses from 0 to 100%. A major variable is introduced due to the difficulty in accurately counting the number of hematopoietic cells. This variable could not be held at a constant, even though unknown, level and was therefore subjected to statistical control by the choice of a statistical design. The design is a partially balanced incomplete-block design which will allow analysis of the major factors after adjusting for variations in number of cells.

Thirteen groups of mice were exposed to one of seven levels of radiation from 0 to 1800 r. Some groups were given protection with *S*,2-aminoethylisothiourea (AET), some with bone-marrow transplants, and some with both; some were given no protection. Diagnoses for each of about 1500 mice were made and grouped into 25 major categories. These results were recorded on punched cards, and summaries of life span and frequencies of incidence of each diagnosis were obtained by the Biomedical Data Recording Unit. Statistical analysis of the effects of radiation on the protected groups as compared with unprotected groups for each category is being performed.

The compounds AET and *S*,3-aminopropyl-*N*′-methylisothiourea were tested in mice as protective agents against radiation damage resulting from 200 to 400 r of x radiation. The procedure used was as follows:

24 hr after an initial x-ray dose with or without chemical protection, the $LD_{50}/30$ was determined by a second exposure to x rays – always without protection. Comparison of $LD_{50}/30$ values showed that under conditions of sublethal total-body irradiation, the compounds tested maintained their protective activity, reducing the radiation effectiveness by a factor of about 1.5 to 2. The effect of x rays on the 24-hr recovery from sublethal radiation injury was determined in mice by utilizing the split-dose technique. Twenty-four hours following an initial x-ray dose, ranging between 100 and 500 r, the $LD_{50}/30$ was measured by a second exposure to x rays. Residual damage was calculated according to the following formula:

$$\frac{LD_{50}/30\ \text{(single dose)} - LD_{50}/30\ \text{(second dose)}}{\text{initial dose}}\ .$$

The residual damage, expressed in percent of the initial dose of x rays, increased progressively with increasing initial dose. The $LD_{50}/30$ values were estimated from least-squares linear regression analysis, where the arc sine of the proportion dying was plotted against dose. Estimates, exact confidence limits, and approximate variances were calculated on an IBM 610 computer.

Health Physics

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ECOLOGY

Fungi and bacteria counts on leaf samples from forest stands were analyzed to test for effects on the counts due to species, season, slope, and elevation. The counts were analyzed by the analysis of variance after use of the square-root transformation in order to make the assumptions for tests of significance valid. The numbers of observations for each combination of factors were not equal but were proportionate, so that an existing program for the IBM 7090 for equal numbers was used in a manner in which the results of several analyses could be combined to get the proper analysis.

CLINCH RIVER STUDIES

Health physicists have continued to study the patterns of concentration of constituents (calcium, chlorides, suspended solids, gross beta radioactivity) in the water of the Clinch River. Previous studies[1] demonstrated the failing of "grab" samples (single samples drawn at random location within the river) to describe adequately the amounts of material carried by the current and the failing of simple experimental designs (such as the simple composite design) to improve sufficiently on the sampling procedure. A more elaborate experiment was conducted at mile 14 on the Clinch River, which is a station approximately ½ mile below Gallaher Bridge.

Here the river is about 500 ft wide and 25 ft deep. At this station a series of 89 samples were taken which were, in general, equally spaced on six concentric ellipses in a vertical plane. Twenty-one of the 89 samples were spaced so as to describe a third-order rotatable design of a type reported by Gardiner, Grandage, and Hader.[2] The four responses, calcium, chlorides, suspended solids, and gross beta, observed at the sample locations are being examined through polynomial regression models at this writing.

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[1] D. A. Gardiner *et al.*, *Math Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, p 31.

[2] D. A. Gardiner, A. H. E. Grandage, and R. J. Hader, *Ann. Math. Statist.* 30, 1082 (1959).

The intent is to discover an appropriate model for describing the patterns of concentration of the constituents and to compare critically the third-order rotatable design with the larger design (of 89 points) as a means of efficiently sampling the river.

WHITE OAK LAKE BED STUDIES

It had been planned to survey the entire White Oak Lake bed to estimate the total amount of radioactivity contained in the soil of its bottom. The nature of the problem demanded a sample survey plan to implement its solution.

The latest, most complete information on the amount of radioactivity in the lake bed was collected according to a systematic plan in 1954. These data were available and were used to devise a stratified sampling plan with optimum allocation of sampling units.

The lake bed was divided into four strata according to the 1954 data. Each stratum represented an area or series of areas in which the observed radioactivity was within an arbitrary interval. The variability of radioactivity within the strata was estimated from the 1954 data. These estimates of variability, coupled with the total areas of each stratum, were used to allocate the proportions of the total sample to the four strata in order to minimize the variance of the new estimate of total radioactivity.

As of December 31, 1961, progress had not extended as far as the determination of sampling locations nor to the collection of samples.

TISSUE ANALYSIS

Statistical consultation was provided to the investigators concerned with the tissue analysis program of the Health Physics Division. The nature of the data is such that nonparametric methods of analysis are more appropriate than the usual parametric statistical techniques. Confidence limits on the median were estimated from tables of the binomial distribution. Rank correlations and associated test statistics were computed by use of the IBM 1620 now available at the University of Tennessee.

INTERACTION OF CHARGED PARTICLES

Some work was done on the problem of interaction of charged particles with a degenerate Fermi-Dirac electron gas. The problem (No. 6.6, p 650 of the reference cited) was presented by Ritchie[3] and has been solved for x and z, with the specific values of χ^2 given. The solutions were a series of near-parabolic curves in the (x, z) plane. A table of these values of (x, z) with the corresponding values of χ^2 was stored on magnetic tape for use with a program now in progress for the evaluation of the interaction probability.

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[3]R. H. Ritchie, *Phys. Rev.* 114, 644–54 (1959).

NUCLEAR-RECOIL-ENERGY DISTRIBUTIONS

The program for calculating nuclear-recoil-energy distribution in a spherical fast-neutron dosimeter previously reported[4] was coded, and its results are being checked.

A BEAM THROUGH A DIELECTRIC MEDIUM

The investigation of a system comprising a beam of charged particles passing through a dispersive medium gave rise to a dispersion equation which can be written as a fourth-degree polynomial.

The study of this dispersion equation by the method as formulated by Sturrack required the plotting of ω-k diagrams. This was accomplished by assigning a value for the frequency ω, computing the coefficients of the fourth-degree polynomial in k, and solving this resulting polynomial. The results have been published.[5]

Similar work is in progress, and several graphs are being drawn which show the numerical values of the parameters of the system for which an instability can occur.

GAMMA-RAY-DOSE CALCULATION

A number of magnetic tapes containing histories of neutrons of varying initial energies followed through a "phantom" body by a Monte Carlo type of method were written and are now in the tape library. These histories will be used as input data for a gamma-ray-dose calculation now nearing completion. The buildup-factor method is being used, which involves placing a number of detectors within the phantom and computing the uncollided dose and collided dose received at each detector from each neutron collision. Each neutron collision is forced to produce a gamma ray, which is weighted accordingly, and each detector is assumed to receive a contribution from this gamma ray according to the detector's distance from the neutron collision site. The uncollided dose is first calculated and then multiplied by the buildup factor to obtain the collided dose. The buildup factor is used as if the phantom were an infinite medium, and therefore the uncollided dose is a lower bound and the collided dose an upper bound on the actual dose received by the detector. These calculations will be used in the study of permissible dosage to humans and animals exposed to radiation.[4]

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[4]D. A. Gardiner *et al.*, *Math. Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, pp 33–34.

[5]Jacob Neufeld and Harvel Wright, *Phys. Rev.* 124, 1–16 (1961).

WHOLE-BODY COUNTER

A program is being written to process data from the RIDL 200-channel analyzer and the nuclear data 512-channal analyzer, which are used to determine radionuclides present in the human body. The data consist of the relative number of gamma rays occurring at energy levels between 0.0 and 1.59 Mev recorded during a given period of time. The present program will strip K^{40}, check the K^{40} scatter band, and strip Cs^{137} from the net spectrum. A semilog plot will be made of the net spectrum and also after each successive stripping. A more complex program, to be written later, will test for as many as six radionuclides.

Metallurgy

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HFIR FUEL ELEMENTS

Probability of Meeting Specifications

A specification (used early in 1961) for the fabrication of the HFIR fuel element stated that of three measurements of the gap between adjacent plates of the fuel element, none could be outside the interval (40 mils, 60 mils). Furthermore, the average of four measurements, one of which was a "free measurement" of exactly 50 mils, could not be outside the interval (47 mils, 53 mils).

Thickness data from 8 fuel plates of a solid type, 15 of a cored type, and 252 fabricated by an independent manufacturer were available for use in determining the probability that the fuel plates could be manufactured to meet specifications if they were assembled perfectly.

The calculations were made on the basis that the data adequately represented the state of the manufacturing art and by assuming a normal-probability density function for the distribution of the measurements. The integrals were evaluated numerically on the Oracle with the following results:

Type of Plate	Probability of Meeting Specifications
Solid	0.597
Cored	0.292
Independently made	0.994

Source and Magnitude of Variability in Channel Measurements

Subsequently an HFIR fuel element was assembled, and measurements were made on the gaps between plates or on the widths of the channels. Measurements were made on 51 inner-annulus channels and 50 outer-annulus channels of the element as originally assembled.

By the analysis of variance the measurements were examined to discover the sources and magnitudes of variability. The model chosen was a mixed model of fixed and random effects containing terms for channels, radial and vertical location of the measurements, and the resulting interactions. Salient discoveries were: (1) that the variation in channel measurements from one radial location to another was greater than from one vertical location to another, and (2) that the act of pulling the fuel element down to size caused even more variation among channel measurements.

Tolerance Limits for Channel Widths in HFIR Fuel Elements

The measurement, X_{ijk}, of a channel width in an HFIR fuel element may be expressed by the model

$$X_{ijk} = \mu + c_i + d_{(i)j} + \epsilon_{(ij)k} ,$$

in which μ is a mean value, c_i is an increment peculiar to the ith channel, $d_{(i)j}$ is an increment peculiar to the jth depth in the ith channel, and $\epsilon_{(ij)k}$ is a random component peculiar to the kth measurement made at the jth depth in the ith channel. A reactor specification states that

$$L_{ij} = (X_{ij1} + X_{ij2} + X_{ij3} + 50)/4$$

must be within the interval 50 ± 3 mils.

Sixty channels were selected at random in an HFIR fuel element, and determinations, L_{i1} and L_{i2}, were made in each channel. Two-sided tolerance limits, T_l and T_u, of the form

$$\text{Prob } (T_l < \text{at least 95\% of all } L\text{'s} < T_u) = 0.99$$

were calculated to shed light on whether the fuel elements could meet this specification; T_l was calculated to be 47.9 mils, and T_u was calculated to be 52.1 mils. Hence the specification appears to be "workable." This may be visualized from the following diagram:

|← At least 95% of the L's →|

47 47.9 52.1 53

Another specification is that each X_{ijk} must be within the interval 50 ± 10 mils. Tolerance limits of the form

$$\text{Prob } (T_l < \text{at least 95\% of } X_{ijk}\text{'s} < T_u) = 0.99$$

were computed, with $T_l = 42.3$ mils and $T_u = 57.7$ mils. The graph of this characteristic is as follows:

|← At least 95% of X_{ijk}'s →|

40 42.3 57.7 60

This specification appears to be workable also.

Probability of Pinholes in a Fuel Element Cladding Penetrating into the UO_2 Particles of the Fuel Matrix

A fuel element is, in its simplest form, a sandwich composed of cladding, fuel matrix (UO_2 particles in matrix alloy), and cladding, in that order. Fuel element fabrication processes, chiefly rolling, cause the cladding, a protective sheath, to develop pinholes of varying diameters and depths. A "leaky" cladding presents a hazard.

Examination of several rolled fuel elements revealed that the depth of the pinholes followed a truncated exponential distribution,

$$f(x) = \frac{1}{\theta} \exp \left[-\frac{1}{\theta} (x - T) \right] ,$$

where x is the depth in microns, T is the point of truncation, and θ is an unknown parameter, which was estimated by the method of maximum likelihood and found to be $\hat{\theta} = 18.44$ for these data.

If the distribution of the number of pits is a Poisson type and if the probability of finding a UO_2 particle in a unit volume is equal to the volume percent of UO_2 in the fuel matrix (25%), the probability of t intersections per fuel plate is

$$\text{Prob }(t) = \frac{1}{4} \left\{ \int_a^b \frac{1}{\hat{\theta}} \exp \left[-\frac{1}{\hat{\theta}} (x - T) \right] dx \right\} \left(\frac{e^{-\lambda} \lambda^t}{t!} \right) ,$$

where t is the intersections per plate, λ is the average number of pinholes per plate, T is the point of truncation (microns), and a and b are the lower and upper limits of penetration (microns). The results of the calculation are shown in Table 1. Thus it is seen that the hazard of exposure of UO_2 particles during fuel element fabrication is small.

Table 1. Probability of t Intersections per Plate

$\hat{\theta} = 18.44$, $T = 50$, $a = 127$, $b = 2.591$

t	Probability when $\lambda = 1.7$	Probability when $\lambda = 1.8$
0	0.0007	0.0006
1	0.0012	0.0011
2	0.0010	0.0010
3	0.0006	0.0006
4	0.0002	0.0003
5	0.0001	0.0001
6	0.00002	0.00003

THORIUM OXIDE PELLETS

Metallurgists at the Laboratory were interested in measuring the effect of time, temperature, and load on the density of thorium oxide pellets formed by hot pressing. A three-factor composite design in two blocks was recommended for the experiment subsequently performed. Each block was run with oxide from a different batch of thorium oxide.

The ranges of the three design variables were: time, 20 to 900 sec; temperature, 1000 to 1600°C; and load, 0 to 3000 psi. The hot-pressed densities varied from 5.36 to 8.42 g/cc.

A quadratic polynomial in the three design variables was fitted to the observations by the method of least squares. Preliminary results indicate a reasonably small deviation of predicted density from observed density. The most important contributor to the hot-pressed density is the temperature under which the oxide is pressed.

The complete analysis, which will involve translations and rotations of the axes in the design space, will be reported in a future publication.

URANIUM-ALUMINUM ALLOYS

An experimental design similar to the one suggested for the thorium oxide study (see above) was selected for examining the effects of annealing time, annealing temperature, and cold reduction on the hardness of aluminum and uranium-aluminum alloys. The design recommended for this experiment was a second-order composite rotatable design. No blocking was necessary. The ranges of the design variables were: annealing time, 1 to 3 hr; annealing temperature, 350 to 550°C; and cold reduction, 0 to 20%. The experiment was performed in triplicate; there was one complete experiment for each of three alloys, and each experiment involved 20 specimens. Six hardness measurements were made on each specimen.

The experiments were completed just prior to this writing, and no statistical analysis has been made as yet. Complete results will be reported in a future publication.

ADVANCED TESTING REACTOR

Selection of a Statistical Design for a Radiation Experiment

In order to present a refined and scientifically complete research proposal to the AEC, the Metallurgy Division requested a statistical design applicable to an in-pile radiation experiment. The purpose of the experiment was to evaluate aluminum-based fuel material for the Advanced Testing Reactor (ATR).

The variables to be investigated, the levels of investigation, and their relative importance to the experimenter are listed in Table 2.

The specimens are to be given a dimensional analysis and a postirradiation examination. Estimated costs are: sample preparation, $100 per sample; dimensional analysis, $200 per sample; and postirradiation examination, $1000 per sample.

It was proposed that a complete 3×2^5 factorial experiment be performed, with all specimens used for the dimensional analysis but with only a one-half replicate of the 3×2^5 factorial used for the post-irradiation examination. This is referred to as design I. An alternative proposal (design II) was to use a complete 3×2^4 factorial experiment, eliminating one of the two-level factors from investigation and including every one of the specimens for both dimensional analysis and postirradiation examination.

A comparison of the effectiveness of the two proposals is given in Tables 3 and 4.

The estimated cost of the proposed radiation experiment for using design I is $76,800, and the estimated cost for using design II is $62,400.

By selecting design I, one may buy, for an additional $14,400, 45% greater efficiency in the study of dimensional effects, information on an additional experimental variable, and have 48 additional irradiated

Table 2. Experimental Variables in the Study of Fuel Elements for the ATR

Variable	Degree of Interest in Variable	Number of Levels
Burnup	Major	2
Cladding	Major	2
Fuel type	Major	2
Temperature	Major	2
Matrix material	Major	3
Poison	Minor	2

Table 3. Comparison of Designs I and II for Evaluating the Effects of Various Factors on the Dimensional Stability of Fuel Elements for the ATR

Design	Number of Samples Required	Number of Factors To Be Investigated	Cost	Relative Efficiency
I (3×2^5)	96	6	$28,800	1.4507
II (3×2^4)	48	5	$14,400	1.000

Table 4. Comparison of Designs I and II for Evaluating the Effects of Various Factors by Postirradiation Examination of Fuel Elements for the ATR

Design	Number of Samples Required	Number of Factors To Be Investigated	Cost	Relative Efficiency
I ($\frac{1}{2}$ of 3×2^5)	48	6	$48,000	0.9837
II (3×2^4)	48	5	$48,000	1.0000

specimens for future examination. The efficiency in studying the effects by postirradiation examination would be only slightly less.

ABSORPTION SPECTRA OF FUSED SALTS

A program was written for the IBM 7090 computer for processing data from absorption spectra of fused-salt studies.[1] The code is divided into two parts. The first part accomplishes the cross-reference indexing, the number conversion, and the storing of data on magnetic tape. The second part locates one or two sets of data stored on magnetic tape and computes a set of spectral information for output. There are four media of output for up to six sets of calculated information to be associated with up to three calculated wave quantities.

In Part I, the spectral information tape (in Grey Code[2]) is transmitted to cards for input on the IBM 7090. The program then converts the Grey Code to its equivalent decimal representation and records it on magnetic tape. Associated with each datum is a wavelength which decreases in equal increments. Along with the record, on magnetic tape, of converted data are written the first and last wavelengths, the increment of wavelength, and the cross-reference identification. A printed copy is made of each record. If spectral data are already available in decimal form, they may be recorded on magnetic tape without passage through the Grey Code conversion.

In Part II, the data are selected from magnetic tape and prepared for output. The output may be a complete set of data or a subset of a complete set. Two sets of spectral information may be combined by subtraction at wavelengths common to both records, and at an increment that is an integer multiple of the least common multiple of the wavelength intervals of the two sets. Prior to output the spectral information may be multiplied by a constant and/or converted to logarithms. The wavelength, wave number, or photon energy associated with each datum is also prepared for output. Output in Part II may be via cards, a printed table, Moseley curve plots, or Oracle curve plots.

MISCELLANEOUS

Statistical Methods Useful in Metallurgical Experimentation

Practical metallurgists frequently introduce a small change in a fabrication process (chiefly rolling methods) and desire to know whether the change results in an improved product. The quality of the finished piece is frequently judged on "appearance," that is, "acceptable appearance" and "non-acceptable appearance." Chi-square procedures or modifications of chi-square methods are suitable in such cases.

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[1] An Oracle program for processing data of these studies was reported in the *Math. Panel Progr. Rept. Sept. 1, 1958, to Dec. 31, 1959*, ORNL-2915, p 26.

[2] The spectrophotometer, which measures the absorption of the fused salts, is equipped with a digitizor which punches the data onto paper tape in a code known as Grey Code.

Memoranda on the following subjects (with illustrated examples) were written as a guide:

1. sample size required to detect a difference between two proportions,
2. comparing two percentages,
3. comparing more than two percentages,
4. some uses of the range in statistical calculations.

Collapse of Tubes by External Pressure

The number of variables affecting the critical pressure for tube collapse requires that master curves of pressure vs the variable be obtained. An Oracle program was written for obtaining the master curves by solving the von Mises equation for the geometric variables length, radius, and wall thickness.

Factorial Experiment for Fuel Element Burnup Study

A 2×4^2 factorial experiment was designed for experimenters of the local MIT Practice School in order to investigate the effect of burnup atmosphere, specimen length, and radiation dosage on Zircaloy pellets. It was recommended that all the pellets be clad uniformly. However, if it should become necessary to investigate the effect of two different claddings, the design could be "blocked" into two parts to accommodate the additional variable. This device confused the clad-by-atmosphere interaction with the length-by-dose interaction.

Reactors

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SISYPHUS

A new nuclear burnup code called SISYPHUS has been written to calculate the fuel composition as a function of time in a homogeneous reactor with no continuous fuel reprocessing. This code is designed to calculate fuel costs as a function of time with a continuous feed of fuel to the reactor and to determine the economically optimum time to operate the reactor before reprocessing the fuel.

The economics calculation is designed to calculate fuel costs at successive flux-time increments, with the nuclear calculation determining fuel compositions and additions or removal of fuel from the core to maintain criticality. The calculation continues until the curve of fuel cost vs reactor operating time passes through a minimum. The individual items making up the total fuel cost are printed out at this optimum point.

Shortly after this version of the code was satisfactorily completed, it became apparent that the code was not versatile enough to handle all situations of interest. For example, the code would calculate the rate at which fuel must be added to the reactor to maintain criticality, but it was not capable of determining a fuel removal rate for the case of breeder reactors. Also, no provision had been made in the economics calculation for including interest charges on operating capital in the reactor fuel cycle.

The calculation was revised, and considerable reprogramming was required to include these items. This modified code is still being debugged.

MODIFICATION TO THE EXPIRE REACTIVITY LIFETIME CODE

The reactivity lifetime code, EXPIRE,[1] was written for use in survey-type reactor calculations needed for reactor optimization. In its original form, the program required a considerable amount of preliminary calculations to generate input data. For example, three separate machine calculations were needed to obtain the effective neutron temperature and thermal-flux disadvantage factors as a function of fuel enrichment before EXPIRE could be run. Also, the task of writing input to supply nuclear data for each

[1] S. Jaye, *EXPIRE, A Reactivity Lifetime Calculation,* ORNL CF-60-10-138 (Oct. 13, 1960).

condition was quite tedious. To eliminate the tedious and time-consuming preliminary calculations and to minimize input requirements, several codes were modified and added to the EXPIRE code as a subroutine package called NTP3. With the modified code, a minimum of input data is required, and the code automatically calculates the effective neutron temperature, flux disadvantage factors, and average nuclear data, and proceeds through the reactivity lifetime calculation.

ERC-5

The ERC-5 program previously reported[2] was modified so that the equations better describe the reactor state. This new program is called ERC-6 and uses the same input as ERC-5 and produces the same output.

ORR FUEL INVENTORY

The ORR Fuel Inventory Code[3] was improved. Now added to the first section is a sort routine which segregates the shim rods, the experimental elements, and the damaged elements from the rest of the inventory. In addition, the remainder of the inventory is sorted according to the U^{235} weight and is printed in this improved format. This section can now be put on the machine within seconds of a shutdown of the ORR. Improved error detection features have been added, resulting in only one rerun this year, and this was due to a personnel error.

The next section has not yet been completed. Many methods of selection have been tried and found unusable. At present, a method which has proved usable in practice has been partially programmed. In essence, it is still a matching method which minimizes errors progressively. Solutions are being reached by hand computation, with an adaptation of the method, in 20% of the time formerly required and with much better accuracy.

ESCAPE OF FISSION PRODUCTS

The program for escape of fission products[4] was completed. The program uses the Crank-Nicholson method for the solution of simultaneous differential equations. In addition to this program, a routine for sorting and evaluating data obtained from this program and other sources was written. Also, modifications were made to the first code; they will allow for a coated fuel element and also for a diffusion coefficient which varies with distance from the center of the fuel element rather than remaining constant. A new program which will combine all these programs is almost completed. In this new program, grid size will be more flexible due to the increase in memory capacity of the IBM 7090 over the IBM 704. Also included will be a routine for an analytic solution of a one-member equation having a constant diffusion coefficient.

[2] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960,* ORNL-3082, pp 34–35.

[3] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960,* ORNL-3082, p 35.

[4] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960,* ORNL-3082, p 36.

SODIUM MASS TRANSFER

The Sodium Components Development Program Working Group of the USAEC has been sponsoring research efforts in sodium mass transfer. Recently, members of the working group requested and received statistical consulting assistance. This assistance consisted of aid in the interpretation of solutions obtained by multiple-regression techniques and counsel in the planning of experiments.

REACTOR END CAPS FOR THE NS "SAVANNAH"

Reactor end caps are classified as either acceptable or nonacceptable. The problem was to test the hypothesis:

$$H_1: \; p \leqq p_1 \,,$$

$$H_2: \; p > p_2 \,,$$

where p is the unknown proportion of nonacceptable end caps in the lot.

$$p_1 = \frac{1}{14{,}544}\,,$$

$$p_2 = \frac{11}{14{,}544}\,,$$

such that

$$\text{Prob (rejecting } H_1 \text{ when } p = p_1) = \alpha = 0.01\,,$$

$$\text{Prob (accepting } H_2 \text{ when } p = p_2) = \beta = 0.01\,.$$

Since rejection results in 100% inspection of the lot, only the equation of the acceptance line was determined as given below:

$$d = -1.916 + 0.0002868n\,,$$

where

d = number of low-cobalt (nonacceptable) end caps found in the sampling and analysis effort,

n = number of end caps to be sampled.

This means that if no defects are found in the first 6681 randomly selected end caps the entire lot may be accepted. If one low-cobalt end cap is found, the sample size would increase to 10,168. If more than two rejects are found, the entire lot must be 100% inspected.

Physics

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OPTICAL PHYSICS

In many problems involving the emission and absorption of light by excited gases, it is necessary to know the electric dipole matrix elements for transitions between various stationary atomic states. The experimental information on such matrix elements, conveniently expressed as dimensionless parameters, the so-called "oscillator strengths" for the transitions, is rather sketchy, and the best available analytical scheme for estimating the desired parameters is often inaccurate or inapplicable. Because of the needs of the optical physics program for reliable estimates of oscillator strengths, an IBM 7090 program is being prepared to supply such estimates.

It is necessary to obtain reliable values for the loss factors and phase-shift factors per pass in simple optical resonators (optical masers); these resonators consist of light paths filled with excited gas and bounded by suitable end reflectors. Such systems allow normal modes at optical frequencies, which correspond to various patterns of excitation on the end reflectors. In order to obtain quantitative information on these modes, an IBM 7090 program was undertaken to calculate the mode shapes and the complex eigenvalues that characterize the mode.

NEUTRON CROSS SECTIONS AND RESONANCE PARAMETERS

Two programs for analyzing transmission data to obtain the parameters of neutron resonances were written for the IBM 7090 computer. The first program is a shape analysis for determining the resonant energies, the total widths, and the neutron widths of the resonances. This program analyzes the transmission data for as many as six resonances at once. The second program is an area analysis for determining the neutron widths of the resonances for assumed total widths. This program analyzes transmission data containing as many as 20 resonances at once. A complete description of the mathematical techniques of analysis and the high-speed computer programs was written as a Laboratory report.[1]

[1] Susie E. Atta and J. A. Harvey, *Numerical Analysis of Neutron Resonances*, ORNL-3205 (Dec. 26, 1961).

In connection with research on neutron capture by activation techniques, a list of definite integrals was evaluated which required cross sections of several elements. Table look-up and interpolation were used to obtain cross-section values. The integrations were performed by applying Simpson's rule for intervals h and $2h$ and then computing the improved approximations.

The program for computing resonance parameters from low-energy neutron cross sections of fissionable nuclei[2] was checked out on the IBM 704–7090 compatibility package. A copy was made of the magnetic tape containing the program, and duplicate card decks were produced of all codes and subroutines used to compile the final program. This information and a description of its use were sent to N. J. Pattenden.[3]

MÖSSBAUER SPECTRA

Calculation of the velocity spectrum for the Mössbauer effect[4] involves the folding of the gamma-ray emission spectrum with the absorption cross section. The general form of the integral is

$$M(x) \approx \int_{-\infty}^{+\infty} I(y + x)\, [1 - e^{a\sigma(y)}]\, dy \; ,$$

where both $I(y + x)$ and $\sigma(y)$ are sums of Lorentzian curves. This code was written in order to obtain a theoretical fit to experimental data, by use of the Mössbauer nucleus Ni^{61}. However, the code may be used to calculate the velocity spectrum for any other Mössbauer nucleus by simply supplying the pertinent information for that nucleus, for example, spins, magnetic moments, applied magnetic fields.

LOW-TEMPERATURE PHYSICS

Several computations have been required in connection with a study of the hfs splitting of Au^{197} alloyed in iron, cobalt, and nickel.[5] Wave functions, x, and integrals involving x for x having 1, 2, or 3 nodes and for angular-momentum values 0, 1, and 2 were computed. The functions $x(r)$ interior to the nucleus are given in terms of spherical Bessel functions; outside the nucleus the wave functions are spherical Hankel functions. Each wave function and its derivative are required to be continuous at the match point.

A variety of nonlinear fittings have been made to find automatic methods for determining various physical constants from the raw data.

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[2] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960,* ORNL-3082, p 38.

[3] Associated with the fast-chopper group of the Physics Division during 1960, from the Atomic Energy Research Establishment, Harwell, England.

[4] H. H. F. Wegener and F. E. Obenshain, *Z. Phys.* **163**, 17 (1961).

[5] L. D. Roberts and J. O. Thomson, *Phys. Div. Ann. Progr. Rept. Feb. 10, 1961,* ORNL-3085, p 69.

INTERNAL-BREMSSTRAHLUNG STUDIES

Two experiments were carried out concerning the internal bremsstrahlung in the beta decay of He^6 (ref 6). The first was designed to measure its ratio to total beta emission and the second to determine the shape of its spectrum. Data from several hundred runs were punched on cards so that the IBM 7090 can be used in final evaluation of the data. Energy calibrations and resolution studies of the internal-bremsstrahlung detector were made by taking spectra of various gamma-emitting sources. Data from these spectra were converted to Moseley integers and plotted on the Moseley curve plotter.

The Coulomb correction to the photon spectrum accompanying beta decay for an allowed transition was computed by use of the expressions derived by Lewis and Ford.

INELASTIC-SCATTERING CROSS SECTIONS

A pilot calculation was coded for the IBM 7090 in order to investigate the strong coupling of two nuclear levels,[7] a ground state 0^+ and a first-excited state 2^+. Four coupled differential equations are to be integrated with a simple parametric form chosen for the coupling functions. The set of equations is integrated four times numerically, each time with different initial values at the origin. The four independent solutions for each of the four radial functions are then superposed to yield the true wave functions. The superposition coefficients are determined by setting up an 8×8 complex matrix equation which matches the internal nuclear functions and their derivatives to the known free-state Coulomb wave functions. For charged particles the calculation gives the total absorption cross section, the total inelastic cross section, and the elastic and inelastic differential cross sections. For neutrons the total nuclear and the total elastic cross sections are also obtained.

Work on two further codes is nearing completion. One is along the same lines as the pilot code but includes a second excited state of spin-parity 4^+. The other code is designed for the study of nucleon elastic scattering and includes spin-orbit coupling.

NUCLEAR PHYSICS AND INSTRUMENTATION

The interaction of a neutron with the doubly closed shell nucleus, Pb^{208}, should be approximately described by assuming that the Pb^{208} nucleus acts as if it were an average potential well. The Schrödinger equation is solved for this well, which is taken to be of the Woods-Saxon form,

$$V(r) = -V_0\left(1 + \exp\frac{r - R}{A}\right)^{-1} .$$

[6] J. K. Bienlein and Frances Pleasonton, *Progress Report*, Jan. 8, 1962.

[7] B. Buck, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1961*, ORNL-3193, p 254.

The parameters are adjusted to give the position of the $4s_{1/2}$ state of Pb^{209} and the $s_{1/2}$ scattering phase shifts.[8] By adding a spin-orbit term (Thomas form) to the potential in order to give the energy position of the $2g_{9/2}$ state, one calculates the width for a virtual $2g_{7/2}$ state at 1.75 Mev. For the diffuseness parameter, $A \sim 0.5 \times 10^{-13}$ cm, this width is 80 kev, or about eight times the observed width of a $j = 7/2$ resonance at this energy.[9]

The original program[10] for calculating ion trajectories in electrostatic fields was completely recoded. Potential values are now computed on the IBM 7090 and stored on magnetic tape. In order to trace the charged particle, second- and fourth-order interpolation was employed on the potential values. Some good results were obtained by using simple electrostatic fields and smooth ion-emitting surfaces.

Codes for predicting the response of gamma-ray scintillation counters[11] were modified to calculate the pulse-height response function of glass liquid scintillators[12] for various geometrical configurations with cylindrical symmetry. Calculations for monoenergetic sources of 0.3 to 10 Mev were carried out.

The code for calculating the pulse-height distribution of light pulses due to gamma-ray interactions in a liquid-scintillator tank was modified for use on the IBM 7090, and several sets of input were run. The code was written to study the observed gamma-ray pulse-height distributions from coincident gammas of varying energy in neutron radiative capture cross-section experiments.[13]

A program was written which will calculate and output Clebsch-Gordan, Racah, and Z coefficients[14] along with their input parameters. The subprograms, called CLEBSH ($l_1\, l_2\,$L; $\alpha\beta$), RACAH ($l_1\,$J$_1\, l_2\,$J$_2$; SL), and Z CØE ($l_1\,$J$_1\, l_2\,$J$_2$; SL), are very similar to routines written by Kostigen.[15]

Angular distribution functions $W_k^I\ (\theta)$ (ref 16) were calculated for $\theta = 0\ (5°)\ 90°$; $K = 1/2, 3/2, 5/2, 7/2$; and $I = K\ (1)\ 7/2$.

EFFECT OF DELTA RAYS ON SCINTILLATOR RESPONSE

In order to obtain an estimate of the fractional energy loss of the primary particle deposited by delta rays outside a cylindrical column, a computer program was written. Results will be compared with experi-

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[8] J. L. Fowler, *J. Tenn. Acad. Sci.* 36, 109 (1961).

[9] J. L. Fowler and E. C. Campbell, *Bull. Am. Phys. Soc.* 6, 251 (1961).

[10] *Phys. Div. Ann. Progr. Rept. Feb. 10, 1960*, ORNL-2910, p 74, and *Math. Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, p 39.

[11] C. D. Zerby and H. S. Moran, *IBM-704 Codes for Predicting the Response of γ-Ray Scintillation Counters*, ORNL CF-60-5-72 (May 1960).

[12] R. L. Macklin, *Naphthalene Derivative Scintillators and Glass Loading Possibilities*, AERE-R3744 (June 1961).

[13] J. H. Gibbons *et al.*, *Phys. Rev.* 122, 182 (1961).

[14] For definitions of these functions see, e.g., M. E. Rose, *Elementary Theory of Angular Momentum*, pp 12, 32, and 107, Wiley, New York, 1957.

[15] T. J. Kostigen, *Fortran II Function Subroutines for Clebsch-Gordan and Racah Coefficients*, XDC 61-1-10 (Jan. 27, 1961).

[16] For a definition of $W_k^I\ (\theta)$ see, e.g., L. Wilets and D. M. Chase, *Phys. Rev.* 103, 1296 (1956).

mentally derived values.[17] Since there is no well-defined theory applicable to the problem, the approach adopted was to employ various approximate methods, of which several should overestimate and one should underestimate the answer.

For the first upper-limit estimation the delta rays are treated as originating from a line source and are assumed to stop in the crystal according to a chosen distribution function. In this case evaluation of a double integral is required. If a point isotropic emission of delta rays is assumed, one equation for the energy loss is obtained which involves a triple integral. This formulation leads also to an overestimate.

By assuming that the delta rays preserve their original direction throughout their entire trajectory, the expression for delta-ray energy loss involves a double integral whose lower and upper limits are the lower and upper limits of a transcendental equation. This expression should provide an underestimate.

A final approach to the problem starts from a basically different method and adopts the results of previously published energy-deposition functions applicable to the slowing down of electrons in various media. The IBM 7090 program made use of the existing Gaussian integration subroutines.

REACTOR POWER SPECTRUM ANALYSIS

The power spectrum of a nuclear reactor is the Fourier transform of the time track of the neutron-density fluctuations. It has been shown that the power spectrum is proportional to the amplitude of the reactor transfer function.[18] The transfer function yields the value of some useful reactor kinetics parameters. Analysis of this type is in progress at both the Bulk Shielding Reactor and the ORR. A program was written to compute the amplitude and phase angle for any harmonic of a function known at a set of equally spaced points. The code was written for the Oracle, with the number of points limited to 800 or less, since all storage is internal. If equipment can be devised to facilitate the gathering of data, the code will be rewritten for the IBM 7090 to utilize the larger storage capacity. The error seems to be small for harmonics lower than the kth, where k is the number of points, but becomes progressively worse for harmonics higher than k.

FISSION-GAS RELEASE

In order to determine the rate of fission-gas release from ceramic fuel materials, the neutron-activation technique was used. The technique consists of a short low-temperature irradiation followed by an out-of-pile high-temperature heat treatment.

From raw data, including total Xe^{133} activity, the fraction of xenon released was calculated as a function of the time of the heat treatment. The rate of diffusion of xenon in the fuel material was calculated and plotted as a function of time and the square root of time.

[17] For a more detailed discussion, see A. Meyer and R. B. Murray, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1961*, ORNL-3193, p 74.

[18] M. N. Moore, *Nuclear Sci. and Eng.* 3, 387 (1958).

DIFFUSION PARAMETERS

To determine diffusion parameters in a variety of moderators from pulsed neutron measurements,[19] a routine was written to make use of the regression code in an iterative method for computing the parameters. The scheme adjusts the diffusion parameters and the transport cross section of the moderator until successive approximations are sufficiently close together.

SHIELDING RESEARCH

A general Monte Carlo program, ØGRE (ref 20), has been written for studying the transport of gamma rays and is now in the preliminary production stage. Gamma-ray histories are written on magnetic tapes which may then be processed as needed. An investigation of the efficiency-cost values for some of the Monte Carlo subroutines indicated the need for FAP tape-handling subroutines. Reading and writing of binary tapes for this program are performed through buffered storage so that tape handling and computation are done simultaneously.

Work has begun on automatic procedures for coupling various shielding codes by use of a standard BCD card output.

SHIELDING FOR HIGH-ENERGY RADIATIONS

A general output code was written to analyze the output from the intranuclear cascade program written by Bertini.[21] The code analyzes the cascade particle output and calculates cascade cross sections for the emission of any combination of emitted particles, provided that the total number is less than ten emitted particles per incident particle. It can also compute the average number, per incident particle, of each of the cascade products considered: protons, neutrons, and each of the three pi mesons. In addition, their energy and angular distribution, as well as excitation energy and angular and momentum distributions of the recoil complex nucleus, can be computed.

Output routines have been written for a program which computes flux levels and energy depositions, in elements or mixtures, resulting from electron-photon cascades initiated by either charged particles or by photons.[22] In this program, source energies may range from 10 Mev to 50 Gev. Targets, of infinite dimension in coordinates normal to the source beam, may be of finite or infinite thicknesses and may comprise a variety of symmetric volume elements.

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[19] E. G. Silver and G. deSaussure, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1961*, ORNL-3193, pp 215, 223.

[20] M. B. Emmett and S. K. Penny, a detailed report on ØGRE is to be published.

[21] H. Bertini, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1961*, ORNL-3193, p 323.

[22] C. D. Zerby and H. S. Moran, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1961*, ORNL-3193, p 329.

Chemistry

D. A. Gardiner   M. M. Goff   Mary J. Mader   Katherine O. Martin

BERYLLIUM OXIDE IRRADIATION EXPERIMENTS

A very large experiment for studying the damage done to BeO pellets by irradiation is being designed. Originally the experiment was designed to study the effects of six variables on pellets of ORNL and French origin.

Subsequently, it became known that there would be insufficient pellets of French origin to do the job properly, and the design had to be revised. The current design deals with ORNL pellets only; those from France will be treated in an auxiliary and independent experiment.

The design variables consist of three fabrication variables and three treatment variables. The fabrication variables, each controlled at two levels, are (1) pellet size, $^1/_4$ and $^1/_2$ in.; (2) grain size, small and large; and (3) density, 90 and 96% of theoretical. The treatment variables are exposure time in the reactor, temperature, and neutron flux. Exposure time and temperature are two-level factors (low and high). Neutron flux has many levels; the flux that a pellet receives depends on its position in the reactor.

The irradiation will be performed in the Engineering Test Reactor at Idaho Falls. There will be four multicapsule assemblies inserted into a 3-in. lattice position in the reactor. Each multicapsule assembly will contain four capsules of pellets, the pellets being stacked. Two capsules in an assembly will be controlled at one temperature and two at another. Two assemblies will contain $^1/_4$-in. pellets, and two will contain $^1/_2$-in. pellets. Two of the assemblies will be irradiated for half the time of irradiation of the other two.

Two hundred eighty-eight pellets will be irradiated; these are divided into six groups of 48 pellets each so that a different battery of postirradiation examinations may be performed on each group. A complex problem of the design is the allocation of the pellets to positions in the capsules so that the neutron fluxes received by the pellets are representative and are balanced both within and among the groups of 48.

CRYSTALLOGRAPHY

Codes for the computation of the absorption correction factors for single-crystal diffraction[1] measurements were written, OR ABS for the Oracle and 9 ABS for the IBM 7090. Subroutines for solving systems

[1]W. R. Busing and H. A. Levy, *Acta Cryst.* 10, 180 (1957).

of equations by Gaussian elimination and for finding coordinates of the corners of a convex polygon, given the faces of the polygon, were written for application in the absorption code.

For use with the automatic defractometer, Oracle and IBM 7090 programs were written for calculating angle settings and for processing spectrometer data. Given a crystal and its orientation, the control program calculates the angle settings at which reflections may be observed. The Oracle program produces a paper tape to be used with the spectrometer.

The processor program takes data punched at the spectrometer and then calculates intensity, background, center of peak, and analyzing time for the setting of angles and the taking of data. Further changes in this program are still anticipated.

A crystallographic least-squares program, ORXLS,[2] which was originally written in SAP language for the IBM 704 and later modified and recompiled for the IBM 7090, was rewritten in the FORTRAN language. This will make the program more understandable and easier to modify. The program may be run on any machine for which FORTRAN translations are available.

MISCELLANEOUS COMPUTATIONS

A program was written for the calculation of the angular distribution of the center-of-mass vectors for beams colliding at any angle.[3] Another code, written for the same Laboratory group but for a different type of problem, calculates partial vapor pressure and performs a least-squares fit to the experimental data.

GAMMA-RAY ATTENUATION EXPERIMENTS

In gamma-ray scintillation spectrometry it is necessary to eliminate interference from beta particles by interposing an absorber between the source and the scintillation detector. This absorber also attenuates the gamma-ray beam slightly, and a correction for this effect is required whenever precise measurements of gamma-ray intensities are to be determined. Although this correction may be computed, direct measurement is preferred because of the geometrical arrangement used. Therefore a series of standard gamma-ray spectra in the energy range 0.022 to 1.83 Mev have been determined by G. D. O'Kelley and T. E. Smith, with interposed absorbers of 0.168 to 4.013 g/cm^2 surface density.

The data are being analyzed with an IBM 7090 program which performs a least-squares fit to the Gaussian full-energy peak of each set of data and obtains the peak area. A correction factor (peak area with no absorber divided by peak area with absorber) is computed for each absorber at each gamma-ray energy used, and a value of the gamma-ray absorption coefficient, μ, is derived.

[2]W. R. Busing and H. A. Levy, *ORXLS, A Crystallographic Least Squares Refinement Program for the IBM 704*, ORNL CF-59-4-37 (April 1959).

[3]S. Datz, D. R. Herschpach, and E. H. Taylor, *J. Chem. Phys.* 35, 1549 (1961).

MOLTEN SALTS

In the Molten-Salt Reactor an $LiF \cdot BeF_2$ mixture will be used as a solvent for the fuel and as the coolant. It is important to know how much oxygen (as oxide) is contained in the salt, and so it had been customary to prepare samples of the solidified mixture and submit them for analysis.

The oxides were measured by a method involving high-temperature fluorination with potassium bromotetrafluoride, with a precision reported to be measured by a coefficient of variation of less than 5%.[4] During the first half of 1961 it became apparent that the variability in the results of the analyses was excessive and that an investigation was in order.

Accordingly, an experimental design of the factorial type was drawn up which would isolate for measurement such possible sources of systematic error as day-to-day variability, variability between morning and afternoon analyses, operator differences, differences between rigs, and differences among the positions within a rig. When the designed experiment was partially performed it became apparent that the design was overly ambitious. It was decided to terminate the experiment in order to learn what could be learned from the results which had been collected. By employing missing-plot techniques in the analysis of variance, the data were analyzed and these conclusions were reached: (1) None of the sources of systematic error could be judged significant at a reasonable probability level. (2) The standard deviation of the process, instead of being about 50 ppm oxygen (corresponding to a coefficient of variation of 5%), was somewhere between 250 and 300 ppm.

Possible causes for this excessive variability advanced by the analytical chemists were that the operators were under pressure and that too much was expected of the equipment in too short a time. Subsequently, the method was used to determine the oxides in some samples of U_3O_8 supplied by the National Bureau of Standards, and the results showed a precision in much closer agreement with the precision claimed by the developers of the method. This suggested that the size of the sample and the size of the particles in the sample might have some relation to the precision of the method.

Another experimental design was drawn up to investigate the effects of particle size and sample size on the precision of the method and at the same time isolate the day-to-day variability and the variability among successive determinations on the same apparatus. The suggested design was a partially confounded 2^2 factorial in 12 replications.[5] A schedule which would eliminate pressure on the operators and allow sufficient time for all the equilibria to be established was chosen for running the design.

However, an alternative statistical procedure was selected. This wos a sequential procedure which would determine whether the analytical method could provide the claimed precision for samples of different quantities and different particle sizes. In this procedure systematic errors were considered to be an integral part of the experimental error.

[4] G. Goldberg, A. S. Meyer, Jr., and J. C. White, *Anal. Chem.* 32, 314–17 (1960).

[5] O. Kempthorne, *The Design and Analysis of Experiments*, p 271, Wiley, New York, 1952.

The sequential procedure was designed to decide that the standard deviation of the process, σ, was 50 ppm or smaller, or that σ was not 50 ppm or smaller. The α risk, that is, the probability of rejecting the decision that $\sigma \leqq 50$ when in reality $\sigma \leqq 50$, was set at 0.01. The β risk, that is, the probability of accepting the decision that $\sigma \leqq 50$ when in reality $\sigma \geqq 250$, was also set at 0.01. The sequential procedure requires that samples be taken (i.e., analyses be made) one at a time and that after each sample the standard deviation of the samples be calculated, by use of all the data collected to that time. Then the decision is made to accept $\sigma \leqq 50$, to reject $\sigma \leqq 50$, or to take another sample. A characteristic of this plan is that, on the average, a terminal decision will be made after five samples.

Accordingly, samples of salt of four types were prepared for oxide analysis. These types were:

A Coarse grain, 1.5 g
B Fine grain, 1.5 g
C Coarse grain, 0.75 g
D Fine grain, 0.75 g

The samples were submitted for analysis, and the analytical chemists were asked to analyze them according to any schedule that they desired. The decision to reject the hypothesis that $\sigma \leqq 50$ ppm was made in all four cases. The decision was reached for types C and D after the second analysis, and the decision was reached for types A and B after the sixth analysis.

Members of the Analytical Chemistry Division and the Reactor Chemistry Division are now developing other methods for determining the amount of oxide oxygen in the $LiF\text{-}BeF_2$ mixture.

Isotope Production

H. P. Carter   A. C. Downing   Mary J. Mader   Joan J. Rayburn

CALCULATION OF THE SHIM CONTOURS FOR THE 255° ISOTOPE SEPARATOR

An IBM 7090 program was written to obtain data for shaping the contours of the magnetic pole pieces to be used in the new 255° isotope separator. The novel feature of this program is its ability to iteratively adjust the shape of the pole pieces to obtain the best possible agreement between the desired and the computed values of H_z along the center line. This program made it possible to shape the pole pieces with a high degree of precision at a saving of much time and labor.

The computer program has two parts. The first computes the magnetic potential between pole pieces of specified shape and from this determines the gradient of the potential across the center line, that is, H_z. Advantage is taken of the symmetry of the geometry. On a cross section the surface of a pole piece constitutes an equipotential curve which is part of the boundary of the semi-infinite two-dimensional region in which the magnetic potential must be calculated. The finite-difference problem associated with this boundary-value problem is solved by using the "overrelaxation" technique. The second part of the program iteratively adjusts the shape of this equipotential curve, subject to certain nonlinear conditions, until the computed gradient across the center line approximates the desired values of H_z.

CALCULATION OF ION TRAJECTORIES IN THE BETA CALUTRON

A program has been written that makes possible the analysis of orbits of ions traveling in the electromagnetic isotope separators used by the Isotopes Division. This program calculates the paths of ions originating with a variety of initial conditions, including Z-wise angular divergence. Previously, the distortions produced in the focused image by this type of divergence had not been calculated. This program makes possible an accurate analysis of image aberrations in the calutron and locates the exact cause of these defocusing effects. The code also facilitates any changes that might be made in the optics of these isotope separators.

To make this computation, the results of magnetic-field measurements in the midplane of a calutron were mathematically described as a function of position. By use of this field function across the midplane as a boundary condition, an expansion for the field was written, with the conditions $\nabla \times \vec{H} = 0$ and $\nabla \cdot \vec{H} = 0$. It was then possible to compute trajectories of ions moving in this field.

Oracle Operation

E. C. Long G. H. Stakes S. O. Smith

Operation of the Oracle was on a three-shift five-day-week schedule until the latter part of May, when the machine was turned off for installation of the Oracle-IBM magnetic-tape systems and the CO_2 fire-extinguishing system. Early in July the installation of the tape system had progressed sufficiently that one-shift operation of the computer could be resumed, while the engineers retained one shift for final debugging. Two-shift operation was resumed in July, but in early November a change was made back to one shift because of the light computing load.

Figure 1 indicates the use of the Oracle since 1954; average monthly hours of good computing time are shown. Figure 2 indicates the hours of machine time used by various divisions during calendar year 1961.

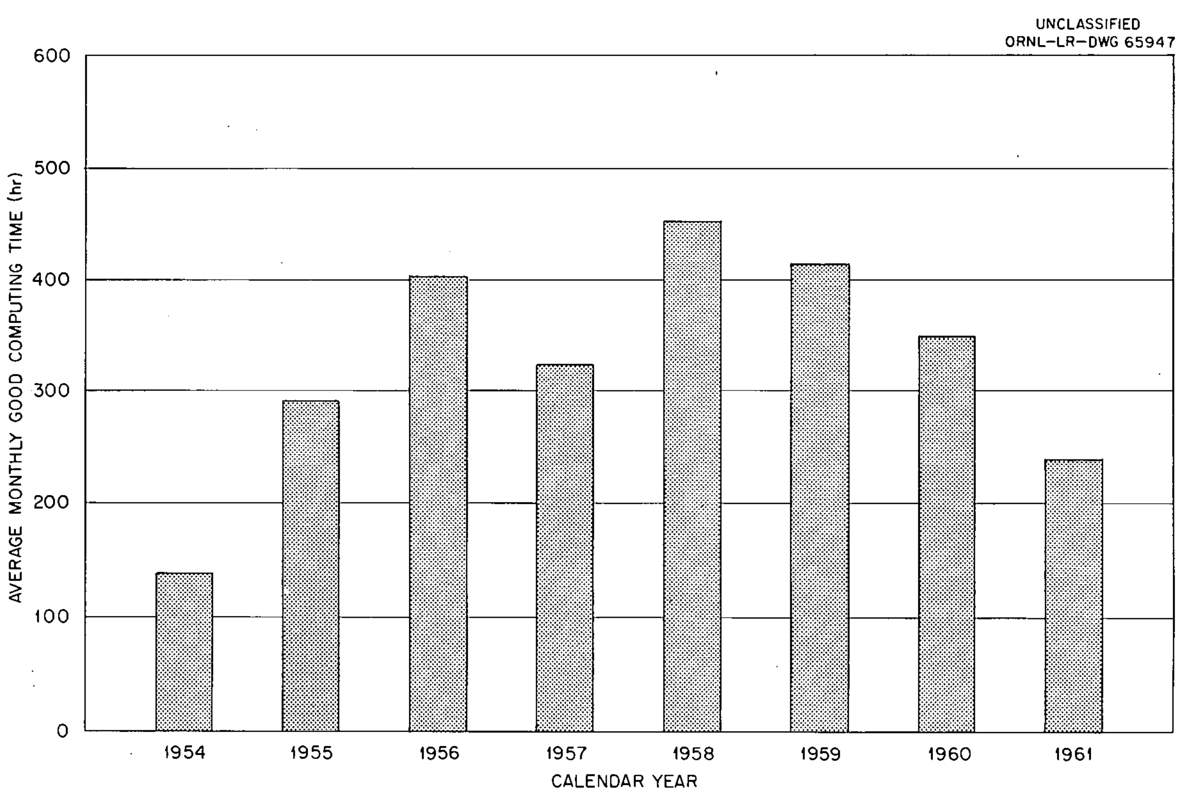

Fig. 1. Use of Oracle Since 1954.

The good operating time and the operating ratio (good computing time/scheduled computing time) are as follows:

Monthly Computing Time (hr)	Operating Ratio (%)
High, 416	97.9
Average, 239	96.1
Low, 105	95.6

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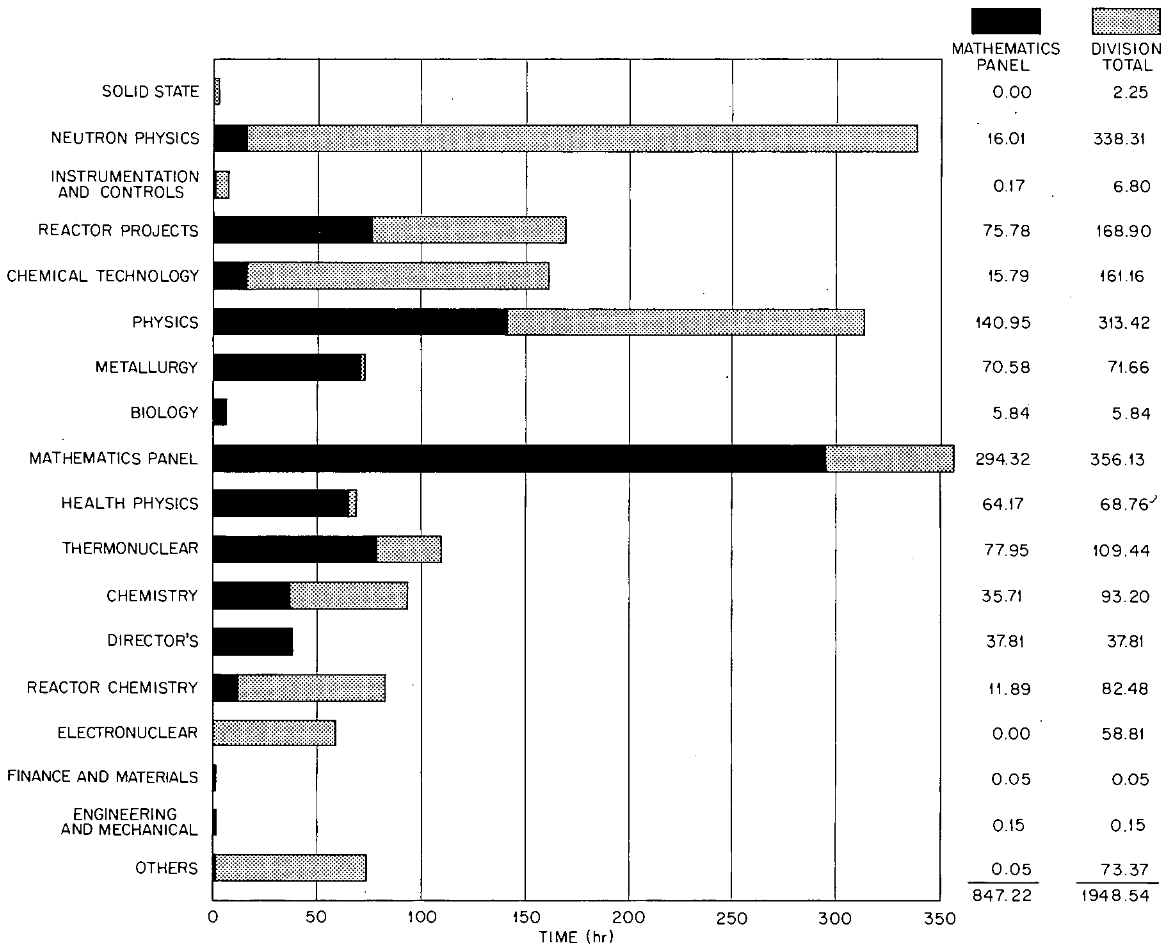

Fig. 2. Oracle Time Used by Divisions During 1961.

Training Courses

LECTURE SERIES

The following lecture series were presented by Manuel Feliciano:

"ORBIT Lecture Series" (intended to introduce beginners to programming techniques using the ORBIT language as a medium), March 1961.

"Introduction to ALGOL" (intended to familiarize a heterogeneous audience with ALGOL 60 and to study techniques which this language makes possible), June 1961.

SEMINARS

The following topics were presented at Mathematics Panel seminars:

D. A. Gardiner

"Experimental Design and Its Application to Research," Metallurgy Division Research Council, June 1961.

"Experimental Design: The Means to Efficient Experimentation," Chemistry Division, July 1961.

"Experimental Design and Its Applications to Research," Health Physics Division, August 1961.

"Design of Experiments," Analytical Chemistry Division, September 1961.

"Design of Experiments," Chemical Technology Division, October 1961.

"Response Surface Methodology," UT-AEC Agricultural Research Laboratory, February 1961.

"Significance Testing," East Tennessee Section, American Society for Quality Control, University of Tennessee, March 1961.

"A Brief Survey of the Design of Experiments from Comparative Designs to Response Surface Techniques," Biology Division, June 1961.

Lectures and Papers

Atta, Susie E. (with J. A. Harvey), "Analysis of Breit-Wigner Resonances," American Physical Society, New York, February 1961.

Atta, Susie E. (with J. A. Harvey), "Shape and Area Analysis of Low-Energy Neutron Resonances," Symposium on Neutron Time-of-Flight Methods, Saclay, France, July 1961.

Carter, H. P., "Careers Through Mathematics," Career Conference, Oak Ridge High School, Oak Ridge, Tennessee, February 23, 1961.

Carter, H. P., "Modern Mathematics in the High School," Workshop for Knox County Mathematics Teachers, Knoxville, Tennessee, August 22–24, 1961.

Carter, H. P., "Computer Facilities at ORNL," Conference on Instrumentation and Technology, ORNL, November 14, 1961.

Dismuke, Nancy M., "Careers in Mathematics for Women," Oak Ridge High School, Oak Ridge, Tennessee, February 22, 1961.

Dismuke, Nancy M., "Some Newer Concepts in Mathematics," Knox County Schools In-Service Education Workshop, Seventh and Eighth Grade Teachers, Knoxville, Tennessee, August 22–24, 1961.

Feliciano, Manuel, "Tarski's Concept of Finiteness," University of Tennessee, Knoxville, February 1961.

Feliciano, Manuel, "ALGOL – An International Algebraic Language," Naval Research Company 6-3, Oak Ridge High School, Oak Ridge, Tennessee, October 1961.

Gardiner, D. A., "The Use of Statistical Methods in Industrial Research," Auburn University, Auburn, Alabama, January 1961.

Gardiner, D. A., "The Use of Experimental Design in Industrial Research," North Carolina State College, Raleigh, January 1961.

Gardiner, D. A., "Experiences with Response Surface Methodology Applied to the Problem of Radioactive Waste Disposal" and "The Use of Experimental Design in Industrial Research," Johns Hopkins University, Baltimore, Maryland, February 1961.

Gardiner, D. A., "Application of Response Surface Techniques to the Preservation of Mammalian Cells," Bone Marrow Conference, University of Buffalo, Buffalo, New York, August 1961.

Gardiner, D. A., "Use of Experimental Design at Oak Ridge National Laboratory," Philadelphia Chapter of American Statistical Association, Philadelphia, Pennsylvania, September 1961.

Gautschi, Walter, "Numerical Integration of Oscillatory Functions," Meeting of Mid-Southeast Chapter of ACM, Oak Ridge, Tennessee, February 1961.

Gautschi, Walter, "Numerical Integration of Periodic Functions" and "Examples of Numerical Instability," Mathematics Department, Vanderbilt University, Nashville, Tennessee, October 1961.

Gautschi, Walter, "Difference Methods in Ordinary Differential Equations," Department of Mathematics, North Carolina State College, Raleigh, December 1961.

Grau, A. A., "ALGOL Research at Oak Ridge National Laboratory," AEC Computer Conference, LaJolla, California, November 2, 1961.

Harkrider, M. T., "An Application of the Crank-Nicholson Method," Meeting of Mid-Southeast Chapter of ACM, Huntsville, Alabama, July 1961.

Householder, A. S., "Exclusion Regions for Characteristic Roots," Colloquium Series in Numerical Analysis, Case Institute of Technology, Cleveland, Ohio, March 24, 1961.

Householder, A. S., "Localization Theorems for the Characteristic Roots of Matrices," University of Kansas, Lawrence, July 28, 1961.

Householder, A. S., "Automation and Education," Summer Institute for Junior High School Teachers of Mathematics, sponsored by NSF at Washburn University, Topeka, Kansas, July 28, 1961.

Householder, A. S., "Localization of Characteristic Roots," IBM Research Laboratory, New York, October 4, 1961.

Householder, A. S., "Localization Theorems for Characteristic Roots," Massachusetts Institute of Technology, Cambridge, Massachusetts, November 14, 1961.

Kastenbaum, M. A., "A Finite Markov Process with One Reflecting and One Absorbing Barrier," Florida State University, Tallahassee, March 1961; University of Florida, Gainesville, March 1961; Purdue University, Lafayette, Indiana, March 1961; Catholic University, Washington, D.C., March 1961; University of Wisconsin, Madison, May 1961.

Publications

Atta, Susie E. (with J. A. Harvey), *Numerical Analysis of Neutron Resonances*, ORNL-3205 (Dec. 26, 1961).

Bottenbruch, H. H., *Structure and Use of ALGOL 60*, ORNL-3148 (July 12, 1961).

Bumgarner, L. L., *Preprocessing of Procedures in the Oracle-ALGOL Translator*, ORNL CF-61-3-1 (May 15, 1961).

Carter, H. P., "The O5R Code: A General-Purpose Monte Carlo Reactor Code for the IBM 704 Computer," Codes for Reactor Computations.

Feliciano, Manuel, "ALGOL Manual" (ed. by the members of the ALCOR group; acting ed., Richard Baumann), translated from the German.

Gardiner, D. A. (with K. E. Cowser), "Optimization of Radionuclide Removal from Low-Level Process Wastes by the Use of Response Surface Methods," *Health Phys.* **5**, 70–78 (1961).

Gautschi, Walter, "Recursive Computation of Certain Integrals," *J. Assoc. Computing Machinery* **8**, 21–40 (1961).

Gautschi, Walter, "Recursive Computation of the Repeated Integrals of the Error Function," *Math. of Computation* **15**, 227–32 (1961).

Gautschi, Walter, "Numerical Integration of Ordinary Differential Equations Based on Trigonometric Polynomials," *Numerische Math.* **3**, 381–97 (1961).

Grau, A. A., *The Structure of an ALGOL Translator*, ORNL-3054 (Jan. 23, 1961).

Grau, A. A., "Recursive Processes and ALGOL Translation," *Communs. Assoc. Computing Machinery* **4**, 10–15 (1961).

Householder, A. S., "On Deflating Matrices," *J. Soc. Ind. Appl. Math.* **9**(1), 89 (1961).

Householder, A. S. (with F. L. Bauer), "Absolute Norms and Characteristic Roots," *Numerische Math.* **3**, 241–46 (1961).

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ORNL-1435	Period Ending October 31, 1952
ORNL-1498	Period Ending January 31, 1953
ORNL-1588	Period Ending June 30, 1953
ORNL-1662	Period Ending December 31, 1953
ORNL-1751	Period Ending June 30, 1954
ORNL-1842	Period Ending December 31, 1954
ORNL-1928	Period Ending June 30, 1955
ORNL-2037	Period Ending December 31, 1955
ORNL-2134	Period Ending June 30, 1956
ORNL-2283	Period Ending February 28, 1957
ORNL-2652	Period Ending August 31, 1958
ORNL-2915	For Period September 1, 1958, to December 31, 1959
ORNL-3082	Period Ending December 31, 1960