ANL-7280

ANL-7280

MASTER

Argonne National Laboratory

**APPLIED MATHEMATICS DIVISION
SUMMARY REPORT**

July 1, 1965 through June 30, 1966

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

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IN NUCLEAR SCIENCE ABSTRACTS

APPLIED MATHEMATICS DIVISION
SUMMARY REPORT

July 1, 1965 through June 30, 1966

Wallace Givens, Division Director

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PREFACE

The objective of the Applied Mathematics Division is to provide mathematical support for the research and development programs of the Laboratory. This goal is achieved, in particular, by (1) conducting research in applied mathematics, numerical analysis, theory and practice of computation, and design of computers and information-processing equipment, (2) providing mathematical consultation, and (3) operating a computational service, using both digital and analog machines. The Division is prepared to provide mathematical assistance at any stage of the development of a problem from its initial formulation to its final solution.

The Consultation and Research Section is available to assist Laboratory personnel by mathematical consultation, in problem formulation, and in selection of appropriate mathematical and numerical techniques, and to carry out analyses of problems. Members of the Section also carry out their own independent research in various aspects of mathematics and programming. The Applied Programming Section is specifically set up to program digital computing problems for members of other Divisions. The members of this Section generally work from a problem description provided either by the problem originator or jointly by the problem originator and a member of the Consultation and Research Section. In addition, this Section also provides production services.

It is the responsibility of the Systems Programming Section to conduct research in new programming techniques, to develop needed systems and subroutines, and to provide training courses and instruction in programming techniques for the benefit of members of the Division, as well as for other members of the Laboratory. Mathematical algorithms and subroutines are developed by the Numerical Methods Group. The Digital Operations Section prepares machine-input data, schedules machine time, and operates the digital machines. The Analog Group is prepared to assist in the formulation, programming, and running of problems for the analog computer or to accept the problem and carry out these services entirely within the Group.

The functions of the Computer Engineering Section are (applied) computer engineering research, and the development and design of computers and information-processing systems having special application to the nuclear sciences.

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A. Wouk, Northwestern University

APPLIED PROGRAMMING

High Energy Physics Applications

Techniques developed in the creation of programs to process film obtained at the CERN spark chamber in 1962 have been found applicable also to film processing from two other experiments.

APPLIED

Some preliminary work, including development of calibration techniques, has been done toward the processing on the film-scanner CHLOE of data to be obtained from spark chamber experiments to be run during the next fiscal year on the Laboratory's Zero Gradient Synchrotron (ZGS). A further effort was initiated to study and correct non-linear distortions inherent in cathode ray tube flying spot scanners.

MASCOT, a program for track reconstruction for the 70-ton spark chamber, was completed. Included is a fitting procedure to either straight lines or helices. This program, as well as another completed program for kinematic event reconstruction, produces as output a magnetic tape suitable for input to the data summarizing program, SUMX.

CHLOE has been further utilized in a program for determining ionization in bubble chamber tracks. Measuring of bubbles and locating and following of tracks is done with great accuracy; simple tests for bubble distortion have been developed to identify crossing tracks easily.

Physics Applications

A program has been written to calculate, for various models of nuclear charge distribution, the spectral lines and their intensities arising in mesic X-rays. The program is being used to compare these theoretical results with experimental results. Furthermore, a program for a similar problem involving a proton or neutron instead of a meson is being written.

Fifteen years of Argonne meteorological readings have now, by means of a computer program, been reduced to tabular and graphic form and submitted to a fair amount of statistical analysis. A program is being written to test a new two-dimensional model of the atmosphere using data consisting of measurements of the carbon-14 content of the atmosphere.

Programs for the IBM 1130 may be assembled on the Control Data 3600 by the use of a program now being written.

Another program, for the ASI 2100, provides graphic man-machine communications to ease and speed analysis of data.

Chemistry Applications

The correction of pulse radiolysis signals for photomultiplier response requires the solution of a Volterra integral equation of the first kind. Although such problems are inherently unstable, solutions have been obtained by using a matrix approximation which employs a smoothing technique based upon the simultaneous minimization of the residual vector and the second derivative of the solution vector.

Methods have been developed for evaluating generalized Debye functions and transport integrals for the study of phonon scattering of vacancies.

To facilitate measurements of fast reactions in radiation chemistry studies, photographs of oscilloscope tracings are submitted for analysis. Techniques were extended to better ascertain line shapes on film using the CHLOE system and the Control Data 3600.

A program was written to solve the diffusion kinetics problem for specified sets of chemical reactions, rate constants, and diffusion coefficients. The system of partial differential equations was solved using a modified Crank-Nicolson method that gives stable implicit solutions over much larger time steps than could be used with previous methods of solution. Results agreed, within the probable error, with those obtained using an IBM 704 program for a particular set of five reactions.

Work was started on the development of a fitting technique to use in conjunction with a differential equation solver to obtain "best" values for reaction rates for reactions as described above, but without considering diffusion. The rate constants must presently be adjusted by the user and amounts of the various species involved compared with observed values to obtain good fits.

A set of IBM 1620 and CDC 3600 programs were developed for the calculation of magnetic resonance spectra from spin Hamiltonians.

Some work has been done on programs from Lawrence Radiation Laboratory for calculating spectra from an l^n configuration with a one- or two-electron shell.

A program was written to check the coefficients for U^2 , U^4 , and U^6 matrix elements for all f^n configurations, and another for fitting data when convolution integrals are involved.

Additional programs were written and existing programs modified to enable the spectroscopist to classify observed lines.

A facility for fitting with combined Gaussian-Lorentzian functions was added to the program to fit Gaussians or Lorentzians to peaks of spectral data.

Several programs to do Hartree-Fock (-Slater) self-consistent field calculations were adapted for use on the Control Data 3600.

Several 3600 machine language (COMPASS) programs were written to analyze the results of experiments utilizing the Van de Graaff and other accelerators. Such multi-parameter analysis codes compute frequency distributions and other statistical quantities for studies of the products of nuclear fission and the emissions from nuclear reactions.

A program written at Stanford to do trajectory calculations for a magnetic beam spectrometer was adapted for use on the Control Data 3600. This necessitated writing a program to transliterate Burroughs Algol 60 into CDC Algol 60 to handle the many sections of the program that do such things as checking out the magnets.

A technique was developed to calculate smooth numerical derivatives based on observed data for thermoelectric power experiments.

A plotting routine, YOLYPLOT, was developed to produce a complete graph of y or $\log_{10} y$ vs. x from a single call in a FORTRAN program. The Calcomp/DD80 package is used, so that plots may be obtained on either graph paper or 35mm film. In addition, the scaling and axis routines in the Calcomp package have been improved.

Reactor Applications

A major effort has been the design and implementation of the ARC (Argonne Reactor Computation) System. ARC is intended to provide its users with automatic cataloging and retrieval of data together with simple methods of calling for computational modules to act on the data. ARC has been designed to eliminate much of the human intervention that is required in proceeding from calculation to calculation and as such requires vast amounts of storage.

The IBM Operating System for the System/360 contains software programs that enable implementation of ARC within it. A system being produced for the IBM 360/50 currently will provide an environment for one-dimensional reactor calculations. Experience with this system will then be used to direct efforts for the full system utilizing the 360/50-75 to be completely installed at Argonne by July of 1967.

The modules currently being planned for the initial one-dimensional ARC effort include transport and diffusion theory neutronics, criticality searches, a neutron inventory, perturbation based on diffusion theory, a collection of modules for fuel cycle studies, a collection of modules to generate cross section data, and related input and output manipulation routines.

Biology and Metallurgy Applications

Considerable effort was devoted to solving, by finite difference methods, the partial differential equations of fluid flow. The solutions are pictures of stream lines. A different method was used to find an approximation to the boundary conditions of an electric potential field by an analytic function.

Two other applied problems with a distinguishing mathematical form were the calculation of the inverse of the error function and the calculation of the variance of the autocorrelation of a general class of birth and death processes.

A computer simulation of chemical reactions at constant pressure or volume took the form of a minimization problem. Many least-square fitting and data handling problems were completed, as, for example, in crystallographic programs.

Information Processing Applications

Although the Applied Mathematics and Particle Accelerator Divisions and Library Services Department provide most of the problems for this group, requests from a number of other divisions have also been fulfilled. Most of the programs have been written for the peripheral Control Data 160-A or the IBM 1401. Several programs for the Control Data 3600 have made extensive use of the SORT II system, thus enabling group members to become quite well-trained in its use.

Engineering aids developed for the Particle Accelerator Division include a ZGS spare cable index, an electrical drawing index, and a ZGS cross-referencing system for terminal block and relay connections.

A study was made of data acquisition and time-sharing systems, and another in detail of an IBM System/360 acquisition.

Topological properties of self-restricting mazes were investigated, and efforts were directed toward several parts of a system for selective dissemination of library information.

A number of programs were written in the area of data transformation, as in editing paper tape or printing information from paper tape.

The following programs have been completed by the Applied Programming Section in the past year:

B101 ORIENTATION AND ANGLE SETTING GENERATION PROGRAM

This program calculates crystal lattice and instrument (goniostat) constants using least-squares. From the determined constants of the experiment, the program generates the instrument angles, 2θ , χ , ϕ for each $h\ k\ l$ reflection permitted under the various extinctions, octant and angle options selected by the user.

The optional output provides punched card output for an automatic Neutron Diffractometer.

B104 COMPUTER SERVICES REPORT FOR LABORATORY ACCOUNTING

This program prepares a monthly report to the Accounting Department and to the individual laboratory cost centers, itemizing the programming time of AMD personnel and the operation time and performance statistics of the major AMD computers.

B129 PACER - A DIGITAL COMPUTER EXECUTIVE PROGRAM FOR PROCESS SIMULATION AND DESIGN

This program is a CDC 3600 version of a Purdue University program called PACER, which is an executive program to be used with equipment subroutines to do process simulation and design.

B145 GENERATION OF DATA FOR CRYSTALLOGRAPHIC PROGRAMS MET153 AND/OR B114

This program processes the collected crystallographic intensity data to allow correction for the Lorentz-polarization and, if needed, spherical absorption effects. The output from this program may be used as input to B114 and/or MET153 programs.

B155 THEORETICAL NEUTRON CAPTURE CROSS SECTIONS

This program is designed to calculate theoretical neutron capture cross sections using the neutron transmission coefficients generated by the ABACUS 2 program. The mathematical model includes the effect of inelastic neutron scattering and is designed for a neutron energy range from 1 KEV to 2 MEV.

B157 LINEAR REGRESSION OF VAPOR PRESSURE

The constants in the linear relationship between the logarithm of the vapor pressure and the reciprocal of the absolute temperature are determined by a least-squares method. The vapor pressure is computed from measured values of the cell parameters, corrected where applicable for thermal expansion, and experimental data of the displacement of the effusion-cell with temperature. The program corrects for non-linearity, created by an inaccurate zero to the displacement, by seeking a minimum in the standard deviation of the isopleths found by making successive changes in the numerical value of the zero.

B163 FIT TO RESISTIVITY VERSUS NEUTRON DOSE

This program does four fits of electrical resistivity increase as an exponential function of neutron dose at an irradiation temperature of 4.20K.

B166 LEAST SQUARES FITTING OF RADIOACTIVE DECAY DATA

This program is used to analyze data from experiments in which two radioactive isotopes are diffused simultaneously into another material. The ratio of the specific activities of the two isotopes is calculated by this program from the total counting rate as a function of elapsed time.

B168 RESISTANCE CORRECTION FOR BOMB CALORIMETRIC DATA

This program calculates resistance corrections from bomb calorimetric data for given thermometers and bridges.

B169 CHRONOPOTENTIOMETRIC DATA ANALYSIS

This program evaluates and plots several functions of chronopotentiometric data.

B170 COMPUTATION OF REACTION AND DECAY CHAINS

This program solves the set of equations arising from N successive first-order reactions. A simple recursion relationship that represents the solution to the "Bateman Equations" is used.

B171 ERROR ANALYSIS OF QUADRUPOLE LENS SYSTEMS

Let

$$R_x = A + Bx + Cy + D/x + Ex^3 + Fxy^2 + Gxy$$

and

$$R_y = A' + B'y + C'x + D'/y + E'y^3 + F'yx^2 + G'yx$$

Given input sets $\{R_x, w, y\}$ and $\{R_y, x, y\}$, this program will determine, in the least squares sense, the parameters $A, B, C, D, E, F, G, A', B', C', D', E', F',$ and G' .

The code contains options for treating any of the parameters as constants and for making any of the primed parameters in R_y be a fixed multiple of the corresponding unprimed parameter in R_x .

B173 CALCULATION OF FLOW SHEETS FOR ENRICHED ALLOY FUEL REPROCESSING

This program generates a flow sheet for an alloy fuel reprocessing system consisting of a hydrochlorinator and pyrohydrolyser.

B174 CALCULATION OF FLOW SHEETS FOR ENRICHED ALLOY FUEL REPROCESSING

This program generates a flow sheet for an alloy fuel reprocessing system consisting of a hydrochlorinator, pyrohydrolyser, and other associated equipment.

B175 CALCULATION OF FLOW SHEETS FOR A FLUID-BED FLUORIDE VOLATILITY PROCESS

This program generates a flow sheet for a fluid-bed fluoride volatility process.

B176 FLUID BED REACTOR DATA ANALYSIS

This program represents the components of a fluid bed reactor and performs material balances and data reduction calculations.

B177 $UO_2 - UF_6$ PILOT PLANT DATA ANALYSIS

This program represents the components of a $UO_2 - UF_6$ pilot plant and performs data reduction calculations.

B179 FISCAL YEAR JOB CARD REVIEW

This program generates a list of jobs to be cancelled due to inactivity during the fiscal year.

B180 VAPOR PRESSURE CALCULATIONS

The equation $C = ae^{\lambda_1 P} + be^{\lambda_2 P}$ is solved for the pressure P , where a and b are constants, λ_1 and λ_2 are functions of the temperature T , and C are input data.

B182 NITRIDATION OF TITANIUM

This program uses ANLZ013 in fitting input data (w, t) and (w, t, p) to equations of the form

$$w = K_1 + K_2 e^{-K_3 t}$$

and

$$w = K_1 + K_2 e^{-K_3 p^{K_4 t}}$$

respectively.

B183 SIMULATION OF CORROSION

This program evaluates sums of the form

$$\sum_{k=1}^N d_k x(t, a_k, c_k, s_k, b_k)$$

where

$$x(t, a, c, s, b) = -\frac{a}{c} + \frac{1-c}{c} (a + (i-1)cs) + b \left\{ t - \frac{s(((i-1) + (i-2)(i-1)c)s + 2a(i-1))}{b^2} + \frac{(a + (i-1)cs)^2}{b^2} \right\}^{1/2}$$

with the integer i determined by the rule that

$$\frac{s}{b^2} \{((i-1) + (i-2)(i-1)c)s + 2a(i-1)\} \leq t \leq \frac{s}{b^2} \{(i+i(i-1)c)s + 2ai\}.$$

B184 NITRIDATION OF TITANIUM

This program uses the variable metric program ANLZ013 to determine optimal values of X_m ($m = 1, 2, 3, 4$) which minimize the function

$$f(X_1, X_2, X_3, X_4) = \sum_{i=1}^{NP} \frac{S_i}{2} \left(\frac{X_1}{1 + X_2 p_i X_3 t_i X_4} - W_i \right)^2,$$

where NP sets of values $\{W_i, t_i, p_i, S_i\}$ are determined by input. Any of the X_m values can be treated as a fixed constant.

B185 FIT TO MAGNETIC SUSCEPTIBILITY DATA

This program fits the form $X = \frac{C}{T-A} + B$ to data of the form (X_i, T_i) , where any combination of A, B, C may be constant or variable.

B187 MODULATED RECIPROCAL CRYSTAL-LATTICE AND DIFFRACTOMETRIC COMPUTER PROGRAM

The program generates Miller indices, tests for space group extinctions, and calculates interplanar spacings and several basic trigonometric functions essential in diffraction studies. The program uses the concept of generalized reciprocal lattice, which is used to govern all of the possible modes of the modulated reciprocal lattice as well as the fundamental reciprocal lattice.

B188 FLUID BED REACTOR DATA ANALYSIS

This program represents the components of a fluid bed reactor and performs material balances and data reduction calculations.

B189 MODEL FOR PARTICLE MOVEMENT IN FLUIDIZED BEDS

The paths of elements of an ideal fluid set in motion by the passage of an approximately circular cylinder are described. The cylinder is located midway between two parallel walls and moves at a uniform velocity.

B190 DATA ANALYSIS OF THE THERMAL DECOMPOSITION OF PLUTONIUM HEXAFLUORIDE

This routine simulates the thermal decomposition of plutonium hexafluoride and performs data reduction calculations.

B191 STAFF SALARY ANALYSIS - SUPERVISORS INCLUDED

This program performs the same statistical calculations as B122 but eliminates the distinction based on area of responsibility.

B192 EQUATIONS FOR HEAT CONTENT OF URANIUM

Given two sets of coefficients for equations of the form $Y = aT + bT^2 + cT^{-1} + e$, the difference between the equations and the derivative of the difference are found for various values of T.

B194 CHEMICAL EQUILIBRIUM CALCULATIONS

This program determines the equilibrium distribution of species within a system of known elemental composition and at a specified pressure (or volume) and temperature by minimizing the free energy subject to the constraint of chemical balance. The temperature of thermal equilibrium and associated concentrations are found by interpolating thermochemical data.

B198 SINGLE CRYSTAL REDUCTION AND ABSORPTION CORRECTIONS FOR SPECIFIED SHAPES

The program processes the collected intensity data by taking into consideration the required corrections for Lorentz polarization, absorption, background and crystal shape effects.

The output from this program is suitable as input to B114 and/or MET153 programs.

B200 STAFF SALARY ANALYSIS - SUPERVISOR SEPARATE

Given data on scientific staff employees concerning schooling and responsibility, experience, and salary, this program sorts and groups data into tables; and for each column of each table, it computes the salary mean, standard deviation, standard error of the mean skewness, kurtosis, and various salary percentiles.

B201 SURFACE TEMPERATURE PROBE ANALYSIS

Given values of U and R, this program computes

$$I(U,R) = \int_0^1 \left[1 - V - \sum_{n=1}^{19999} \frac{4}{n^2 \pi^2 U} \sin(n\pi V) \left\{ \left[\frac{I_1(n\pi U)}{I_0(n\pi U)} \right]^{-1} + R \frac{K_0(n\pi U)}{K_1(n\pi U)} \right\}^{-1} \right] dV$$

$$= \frac{1}{2} - \sum_{n=1}^{10000} \frac{8}{(2n-1)^3 \pi^3 U} \left\{ \left[\frac{I_1((2n-1)\pi U)}{I_0((2n-1)\pi U)} \right]^{-1} + R \frac{K_0((2n-1)\pi U)}{K_1((2n-1)\pi U)} \right\}^{-1}$$

B202 SURFACE TEMPERATURE PROBE ANALYSIS

This program obtains a table of

$$I(\alpha, R) = 1 - \frac{4}{\pi} \int_0^\infty \frac{\sin \alpha x}{x^2 \left[\frac{I_0(x)}{I_1(x)} + R \frac{K_0(x)}{K_1(x)} \right]} dx$$

for given input values of α and R.

B208 FACTORIAL ANALYSIS SIMULATION

Given up to five numbers $X_i = \pm 1$ and the coefficients, form

$$Z = \sum_{i=1}^5 a_i X_i + \sum_{i<j} a_{ij} X_i X_j + \dots + \sum_{i<j<k<l<m} a_{ijklm} X_i X_j X_k X_l X_m + R$$

where R is a Gaussian random variable with mean zero and given variance.

B214 ENERGY CALCULATIONS FOR A RIGID LATTICE TWIST BOUNDARY

This program determines the boundary energy of a twist boundary in a sodium chloride-type salt.

B215 LEAST SQUARES FIT TO A CUBIC FUNCTION

An option was added to the library program ANLE212 (a program to fit an arbitrary linear function) to permit input of a specified constant term. This program also provides for plotting input and results.

B217 TEMPERATURE CORRECTION FOR BOMB CALORIMETRIC DATA

This program calculates resistance corrections from bomb calorimetric data.

B218 RATE OF REACTION OF TITANIUM WITH NITROGEN

This program determines the optimal values of X_1 , X_2 , X_3 , and X_4 which minimize the function

$$f(X_1, X_2, X_3, X_4) = \frac{1}{4} \sum_{i=1}^{NP} \left\{ .36553 \left(1 - e^{-X_4^2 \sqrt{t_i}} \right) \left[X_1^2 + X_2^2 \left(X_3^2 P_i^{-\frac{1}{2}} \right)^{-1} \right] - W_i \right\}^2 S_i$$

for NP given values of W_i , t_i , P_i , and S_i .

B220 FLUID BED REACTOR DATA ANALYSIS

This program represents the components of a fluid bed reactor and performs material balances and data reduction calculations.

B223

SOLID LIQUID EQUILIBRIA

Given tables of $X_s(T)$ and $X_l(T)$ and input constants R , L_1 , L_2 , T_1 , and T_2 , this program determines the parameters B' and B which best satisfy the equations

$$T = (B'X_s^2(T) - BX_l^2(T) - L_1) / \left(R \ln \frac{1 - X_l(T)}{1 - X_s(T)} - \frac{L_1}{T_1} \right)$$

and

$$T = (B'(1 - X_s(T))^2 - B(1 - X_l(T))^2 - L_2) / \left(R \ln \frac{X_l(T)}{X_s(T)} - \frac{L_2}{T_2} \right)$$

for a given range of T values.

B224

A LEAST SQUARES DETERMINATION OF PARAMETERS INVOLVED IN TEMPERATURE-DEPENDENT FUNCTIONS FOR CELL VOLTAGE

This program performs a least squares fit to two functions for cell voltage.

B225

PARTICLE MOVEMENT IN FLUIDIZED BEDS

The paths of elements of an ideal fluid set in motion by the passage of approximately circular cylinders moving in a chain along the X axis are described. The cylinders are equally spaced and are moving through an infinite medium.

B228

DIFFERENTIAL DOSE CURVES

Given an equation for the irradiation induced electrical resistivity, $\rho = A - Be^{-\alpha t} + Cte^{-\beta t}$ as a function of time, t , ρ and $d\rho/dt$ are calculated and plotted with observed values of ρ and $d\rho/dt$.

B229

CALCULATION OF ENERGY RELEASED IN IRRADIATED MATERIALS

This program evaluates a function $T = f(P_1, P_2)$ for sets of (t, P_1, P_2) and determines dt/dT at every calculated value of T .

B231

STATIONARY RADIAL RADIATION FROM A CYLINDER

This problem consists of obtaining a finite difference approximation to the Laplace equation on a cylindrical rod whose ends are at known fixed temperatures and whose radial radiation follows a fourth and fifth power law.

B233

RING MAGNET POWER SUPPLY SHUNT ERROR VOLTAGES

Error voltages, induced by sheet current spatial disparities in the ZGS Ring Magnet Power Supply Shunt, are calculated by solving one of Maxwell's equations subject to the boundary conditions of the Shunt detector system.

C104 CONSTANT DIFFERENCE OF SPECTRUM LINES I

Given lists of N spectrum lines and M levels with widths and other information for each, this program finds all pairs of the N x N or N x M differences (or sums) which repeat a specified number of times within a specified tolerance. The differences (or sums) of the widths are also furnished and the other information reproduced.

C105 SPACINGS OF ENERGY LEVELS

This program computes the average spacings of the eigenvalues of a matrix and then computes the distribution of the spacings for particular grid factors.

C108 TERM ARRAY

Given a list of N + M terms with widths and other information, this program furnishes an array of all N x M wave numbers within a specified range, with wave lengths and differences in widths. It also furnishes an ordered list of the wave number differences with terms.

C116 RADIATION CHEMISTRY KINETICS CALCULATIONS

Given a set of chemical equations and the associated rate constants, the program generates the system of differential equations relating the concentrations of the various reactants and reaction products. The system is then solved to find, at a given time or at essentially infinite time, the concentrations both of substances originally present and of intermediate and final reaction products. The Adams-Moulton method is used with a Runge-Kutta starter.

C127 PLOT6, PLOTTING PROGRAM (PRINTER PLOTS)

This is a subroutine designed to output up to six curves per call on the standard output unit.

C128 RELATIVE X-SECTIONS OF NUCLEAR REACTION ISOMERS

The program computes the relative cross sections of isomers produced in nuclear reactions. The cross sections of the partial compound nucleus, normalized initial compound nucleus spin distribution, normalized spin distribution following particle emission and normalized spin distribution following gamma ray emission are computed at the user's option.

C130

CALCULATION OF CONFIDENCE INTERVALS

Given ϵ and w , this program calculates confidence intervals (V_u, V_L) according to the following formulas:

$$\text{Case 1: } \int_0^{V_u} P(v|w) dv = .5(1-\epsilon) = \int_{V_L}^{\infty} P(v|w) dv$$

Case K, K=2,3 or 4:

$$\int_{V_u}^{V_L} P(v|w) = \epsilon \text{ and } P(V_L|w + 8 - 2K) = P(V_u|w + 8 - 2K).$$

$$P(v|w) = \frac{v^{\frac{w}{2}-1} e^{-\frac{v}{2}}}{2^{\frac{w}{2}} \Gamma \frac{w}{2}} \quad \text{in all cases.}$$

C137

THERMAL ELECTRIC POWER OF QUENCHED METALS

This program approximates the first derivative of a function $y = f(x)$ from a given set of experimental data points (x_i, y_i) .

C138

TRANSPORT INTEGRALS FOR PHONON DRAG RESISTIVITY

The program evaluates transport integrals for phonon drag resistivity.

C142

CRITICAL IONIZATION CALCULATION FOR RARE GASES

Given mass spectrometer (x, y) data, the program calculates and plots first and second derivatives.

C145

PROGRAM TO EDIT AND LIST CARDS CONTAINING SPECTRAL LINE INFORMATION

This program edits and lists spectral line data cards according to special user-supplied formats. It has been designed to facilitate program modification by the user.

C149

BERYLLIUM FILTER

For given values of the parameters $k, \kappa, \tilde{\kappa}, \omega, \tilde{\omega}$, calculate

$$M(r, t) = \frac{\int_0^{E_c} dx \sqrt{x} e^{x/kT} \frac{\sin \kappa r}{\kappa r} \cos \omega t}{\int_0^{E_c} dx \sqrt{x} e^{x/kT}}$$

Plot 1) $M(r, t)$ and $[M(0, t)(\sin \tilde{\kappa} r / \tilde{\kappa} r)]$ vs. r , and 2) $M(0, t)$ and $\cos \tilde{\omega} t$ vs. t , to compare the periods of the functions.

C150 LINEAR SECOND ORDER RATE LAW PROGRAM

Given the concentrations of reactant A as a function of time, together with the initial concentrations of A and B, the program determines the reaction rate k for the reaction of A with B.

C151 INTEGRATION OF SPECTRAL DATA

Peaks of spectral absorption data are determined by least squares fitting to sums of either Gaussian distributions or Lorentzian distributions or products of the two. Finally the integrals for each peak are computed.

C153 MASS SPECTROMETER DATA PROCESSING OF INTENSITY PRESSURE RELATIONSHIPS

Given sets of Van de Graaff experimental data consisting of peak height vs. pressure information associated with many mass numbers, the corrected intensities are calculated and plotted as a function of pressure for each mass number.

C156 MODIFICATION OF MASTER WAVE NUMBER TAPE

Program deletes lines from the Master Wave Number Tape if they are either less than a certain intensity or if they have already been classified.

C158 WAVE NUMBER COINCIDENCE PROGRAM

This program is a modification of the C108 TERM ARRAY program in that the calculated wave numbers and associated quantities are output only when they are within a specified ϵ of an experimental value.

C159 FURTHER PROCESSING OF MASS SPECTROMETER DATA

Given values of corrected intensities of specified pressures for pertinent mass numbers, the program calculates and plots fractional intensities.

C160 CHECK OF $U^{(k)}$ MATRIX TAPE

The program checks single-particle matrix elements of even-rank tensor operators. The tape was reproduced from C. W. Nielson and George F. Koster, "Spectroscopic Coefficients for p^N , d^N , f^N Configurations," M.I.T. Press, 1963.

C162 SECOND MOMENTS OF EIGENVALUE DISTRIBUTION

The program computes second moments of the consecutive spacings of an eigenvalue distribution.

C163 DUMP OF ENERGY DATA

Binary Data obtained from a multi-parameter analyzer are read in 512 30-bit words per record format and separated into 512 Parameter A, B, C triplets. These triplets are output, as well as an array (C X B) whose entries represent the frequency of particular Parameter C, Parameter B words.

C165 REDUCTION OF NEPTUNIUM (IV) BY EUROPIUM (II)

This is a least squares fitting procedure for A, B, and C in

$$t = A + B \log D + C \log (D - D_{\infty})$$

C166 HARTREE-FOCK PROGRAM

This is a HARTREE-FOCK SCF Atomic Structure Calculation.

C167 INTEQN, CORRECTION OF PULSE RADIOLYSIS SIGNALS FOR PHOTOMULTIPLIER RESPONSE

The correction of pulse radiolysis signals for photomultiplier response leads to a linear integral equation of the first kind. Such problems are inherently unstable, hence difficult to solve. A smoothing technique was used to solve the resulting integral equation.

C169 NP(V) - CR(II) REACTION

This is a least squares determination of rate constants for NP(V) - CR(II) reaction.

C173 THERMO-ELECTRIC POWER CALCULATIONS

The program reads thermocouple data or germanium resistance thermometer data, obtains the corresponding temperatures, and then calculates and plots derivatives of a signal with respect to the temperature.

The program may also be used to calculate and plot derivatives of (X, Y) data as input.

C174 ANALYSIS OF ACTIVATION ENERGY SPECTRUM

The program evaluates two related integrals using Romberg integration.

C175 LEAST SQUARES DETERMINATION OF SLATER PARAMETERS FROM OPTICAL SPECTRA

This program calculates values of Slater parameters giving a best fit with observed energy levels, where each element of the energy matrix is specified as a linear combination of the parameters. Successive least squares iterations are made until the residual converges to a specified tolerance or diverges. The numerical matrix, eigenvalues, eigenvectors, (eigenvectors **2), and g-factors are calculated for each iteration.

C176 SPIN ORBIT CALCULATION

This is a driver and a set of routines to calculate Wigner 3J, 6J, 9J, and 12J coefficients. These routines are part of a set of programs from LRL* to calculate electrostatic and spin orbit matrices in $l^n l^{n'}$ configurations.

C177 HARTREE-FOCK-SLATER PROGRAM

This is a HARTREE-FOCK-SLATER Self-Consistent Atomic Field Calculation.

C182 SCHOTTKY FUNCTION

Calculation of the SCHOTTKY Function for specified temperatures is performed.

C183 LEAST SQUARES FITTING OF DECAY DATA

A sum of exponentials is fitted to a set of measured points.

H102 MASMER

This program produces, updates, and merges Master List tapes which are input to and output from the bubble chamber data analysis programs, particularly HGEOM, HEP 151; GRIND, HEP 124; SUM-X Hill, and SUMTAP, H121.

This program also produces data summary tapes using a master list tape as input.

H104 MASCOT - SPARK CHAMBER GEOMETRY RECONSTRUCTION

MASCOT is a geometry reconstruction program for the 70-ton magnetic spark chamber.

H105 MONTE CARLO GENERATION OF NEUTRAL DECAYS

The program generates events that result from the interaction of a pi-minus particle with a proton in a cylindrical target. Of importance is the determination of the bias inherent in the experimental setup.

*Lawrence Radiation Laboratory

H107 BULLSEYE

This is a Monte Carlo program to determine the neutrino spectrum for pions generated in the horn of the ZGS.* Characteristics of the horn, the decay area, and the neutrino facility may be varied to determine various neutrino spectra.

H112 PRINTAPE

This program reads and prints out BCD summaries of the information stored on Master List tapes which are produced by the bubble chamber data analysis programs.

H113 TRNSLATE (CERN)

The purpose of this program is to read in TITLES data (either on cards or BCD tape) and to print out these data, along with explanatory comments, in an easily understandable form. The program assumes a familiarity with the GRIND system.

H114 VIEW

The purpose of this program is to determine the percentage of the interior of a 12-foot (in diameter) cylindrical bubble chamber which is visible to four cameras.

H115 LANDAU FLUCTUATION ON ENERGY LOSS

A probability distribution of energy loss is calculated for a particle passing through a medium.

H119 SPECTRA

Tables of inverse cumulative distribution functions are computed from experimentally determined distribution functions for pion production in the horn of the ZGS. These tables are incorporated in an interpolation routine for use in a Monte Carlo program.

H125 COPY

This program salvages flawed Master List Tapes produced by the bubble chamber data analysis programs. It reads and copies the Master List tapes, inserting proper end-of-tape records and deleting events where parity errors, insufficient data, and out-of-order records occur.

*Zero Gradient Synchrotron

I103 ZGS SPARE CABLE INDEX

All of the spare cables in the ZGS complex are listed according to building, area and terminal location of the origin and destination of the cables, the cable type and number, and whether the cable is entirely spare or only partially spare. A description of how to use the Index is printed as an introduction to the Index.

I105 PAD ELECTRICAL DRAWING LIST

A sorted index to the large file of PAD electrical drawings is obtained in printed form. Two different sorting arrangements are provided; first, in ascending order by drawing number, and second by drawing size. Some editing and rearranging of input data is done and page numbering and headings are added to present the output in a convenient format.

I107 ZGS CROSS-CONNECT SYSTEM

An index is produced to identify and give cross-referencing for the many connections of terminal blocks and relays used in the ZGS complex. The various columns of printed output are appropriately headed with explanatory information, and pages are numbered. Making modifications as well as updating the entire index or only portions of it is an essential by-product of this program.

I109 FINGERPRINT CLASSIFICATION UTILITY ROUTINE

This utility routine converts sets of information on punched paper tape to magnetic tape. Each set of information is composed of an ID section and a data section. Error checking is performed while reading in the paper tape. The magnetic tape prepared by this routine is used as input to a 3600 program.

I111 EDIT SPECIAL TRANSCRIBE MAGNETIC TAPES

Essentially the program is a tape-to-tape routine with editing capabilities. Each record, with Format (7(A1,2I5), read from the original magnetic tape is checked for format errors and corrected if necessary, then written on the corrected magnetic tape. The original tape was prepared by the 160-A Transcribe Program.

I114 COORDINATE CALCULATIONS

The program will generate rectangular coordinates given various input: origin, radius, radius increment, number of increments, initial angle, etc.; and punch the coordinates on paper tape in one of six formats.

I115

TALLY LIST

The program will list paper tape, punched on a tally device, on the CDC 1612 printer.

The paper tape contains up to 4096 sets of information, each consisting of a channel number followed by the data for that channel.

P113

ZEEMAN SPECTRAL FIT BY VARIABLE METRIC MINIMIZATION

This is an adaptation of Variable Metric Minimization to fit experimental Zeeman spectra to a linear combination of curve forms $y(x)$ where $y(x)$ is an approximation

$$\int_{-\infty}^{\infty} \frac{dz \cdot e^{\frac{-t}{1+z^2}}}{K^2 + (z-x)^2}$$

P120

ANALYSIS OF MAGNETIC SPECTROGRAPH DATA

Determination of the relative intensities and energies of gamma rays in the complex spectra observed following neutron capture in neutron resonances is accomplished. This is an adaptation of 704 program PHY222.

P127

TRANSFER MECHANISMS OF ELECTRONIC EXCITATION ENERGY

This program computes the critical transfer distance and critical concentration for which energy transfer occurs between molecules from the overlap region of the absorption and emission spectra. Spectra for the sensitizer and acceptor have been corrected for instrument response.

P130

MATCHING OF SECTIONS OF FLOOR OF HILBERT DOMAINS

The topological structure of the Hilbert domains is established by matching points on the floor analogous to the matching of sides of a parallelogram to form a torus.

P131

AUTO-CORRELATION OF GAMMA-RAY FREQUENCIES

Auto-correlation of a gamma-ray whose frequency assumes six values in a random manner is computed.

P134

MULTIPLE SCATTERING CORRECTIONS FOR NEUTRON SCATTERING IN THIN PLATES

The objective of this program is to determine the cross section for scattering of neutrons by neutrons of nuclei in thin plates by connecting the observed distribution of counts for the effects of multiple scattering.

P138 INVERSION OF OVERLAP MATRICES FOR CRYSTALS

The overlap matrix for a crystal with periodic boundary conditions is inverted using an algorithm due to Arai (Arai & Gabriel, Phys. Rev., to be published 1966).

P139 SEVEN-CHANNEL PAPER-TAPE-TO-CARD CONVERSION

Raw data on paper tape are converted to cards.

P146 GAMMA RAY SPECTRAL ANALYSIS

The capture of a neutron by the nucleus causes the nucleus to enter an excited state. The excited nucleus then emits this excitation energy in the form of a gamma ray of various energies. Analysis of the energy of sums and differences of the emitted gamma ray gives an indication of the energy states of the nucleus.

Data in the form of fringe numbers are converted into energies and then searched for energy sums and differences that suggest nuclear energy levels.

P148 WEIGHT TABULATION FOR NUMERICAL QUADRATURE FORMULAE

Weights are tabulated for various low orders of a new family of numerical quadrature formulae of the form

$$\int_0^1 f(x)dx = \sum_{i=1}^n H_i x_i.$$

P149 ELEMENTARY STATISTICAL ANALYSIS

The program computes the mean, variance, and standard deviation for a set of measurements.

P150 LEAST SQUARES FITS TO BLOCKING DATA

This program fits a function composed of a linear plus an exponential term to a set of experimentally determined points.

P155 OPTIMUM QUADRATURE FORMULAE

Weights and abscissae are tabulated for a new family of numerical quadrature formulae of the form

$$\int_0^1 f(x)dx = \sum_{i=1}^n H_i x_i.$$

These formulae are optimal among all quadrature formulae of given order when the only requirement of $f(x)$ is that it be analytic.

P166 FLUORESCENCE DECAY TIME

A convolution integral is evaluated and tabular results printed and plotted.

R102 INVERSE KINETICS

Given the space-independent, one-energy-group reactor kinetics equations and initial conditions, this program determines the time variation of reactivity required to produce the given input of flux-time data.

The program has three optional methods of representing the flux, five options for the determination of flux and reactivity derivative and four options for flux smoothing.

A library of delayed neutron data from ANL 5800 Reactor Physics Constants is included in the program.

R105 NEARREX

This FORTRAN program computes energy averages of integrated compound nucleus scattering, capture and fission cross sections.

R106 THERMOS

The scalar thermal neutron spectrum is computed as a function of position in a lattice by solving the integral transport equation with isotropic scattering. One dimensional slab or cylindrical geometry can be used.

R112 ITERATE

This is an iterative method for the unfolding of output data from detection systems.

R117 STABLE-3 (KAPL) HYDRAULIC STABILITY EXAMINATION

This program examines the hydraulic stability of a single boiling coolant channel in parallel with many other channels.

R120 LEGENDREVILLE

This is a least square Legendre polynomial fit written in FORTRAN.

R121 MUSCATONE

This is a FORTRAN program for the processing of fast neutron scattering data.

R128 GHA

R128 is a two-dimensional code which computes the temperature response to power and inlet coolant temperature. The reactivity feedback of the reactor is also computed.

R130 HEAT TRANSFER AND FRICTION FACTOR SUBROUTINE

Using the latest published information, these subroutines (2) were prepared to perform both the friction and heat transfer computations for rough or smooth tube hydrogen flow as well as general heat transfer calculations.

R138 UNFOLD

Numerical solutions of certain integral equations of the first kind are produced.

R142 GAUSSIAN FIT

R142 fits experimental data to the Gaussian curve

$$y = a \cdot \exp \left(\frac{-4(\ln 2)(x-c)^2}{u^2} \right)$$

The area under the curve, the decay-corrected area under the curve, and the disintegration rate are then calculated using the parameters a , u and c .

R145 ORCO

This program is a CDC 3600 version of the RE297, IBM 704 program. The program constructs a least-squares approximation of a neutron spectrum, $\phi(\epsilon)$, as determined from a series of activation measurements.

R148 TEMPERATURE DISTRIBUTIONS IN COLDTRAPS

The temperature and precipitate distributions of a coldtrap are found given the velocity distribution and the inlet temperatures.

R153 AISITE II (AI)

This is a tool for parametric investigation of reactor siting.

R159 REACTOR SYSTEM STATIC CHECK

The program effects a system static check for a reactor design by solving a system of 69 non-linear algebraic equations.

R162 FISSION NEUTRON SPECTRUM

Data for a neutron fission spectrum are fitted to a semi-empirical center of mass spectrum including the effect of angular distribution.

BIM124 CALCULATION OF RADIOACTIVITY IN SAMPLES

This program calculates the radioactivity in samples measured with a 400-channel gamma spectrometer, and uses these initial results to determine the biological and effective retention of the samples.

CHM199 CALCULATION OF ELECTRONIC TRANSITION PROBABILITIES

The program calculates theoretical probabilities for electronic transitions between a ground state of an ionized atom and a large number of its excited states. Two different mechanisms for the transitions are considered, namely electric dipole and magnetic dipole. Also included is an option to fit, by least squares, the results of the electric dipole calculation to various energy levels found in 1849/CHM177.

HEP146A KE2

In the Ke(2) experiment it is proposed to study the decay of a K^+ into an electron and a neutrino. The electron will pass through various experimental devices to determine its momentum. The KE2 program studies the decay of a K^+ in a target containing one or more materials. The effects of range straggling, energy losses and multiple scattering are included in the Monte Carlo simulation. A tape containing sample tracks is generated for use in a program to study the electron trajectories.

HEP146B EPLUS

In the Ke(2) experiment it is proposed to study the decay of a K^+ into an electron and a neutrino. The EPLUS program will follow sample electrons generated from the K^+ decay through an experimental area consisting of Cerenkov counters, spark chambers, and a bending magnet. The effects of multiple scattering, energy losses due to collisions, radiation, and screening, and the presence of a magnetic field are included in the Monte Carlo simulation. A tape containing spark coordinates and a tape containing the location and momentum 4-vector for each particle upon exiting each sector are generated.

LIB101 LIBRARY SERVICES BOOK AND CATALOG MAGNETIC TAPE SYSTEM

This program accepts book and catalog information which has been punched onto cards by the Library Services Department and

1. Edits the data deck.
2. Creates a Master File on magnetic tape from the data deck.
3. Prints the Master File.
4. Updates the Master File.
5. Produces an Author File, a Title File, and a Subject File from the Master File.

PAD144 A MORPHOLOGY OF SOME SYSTEMS OF QUADRUPOLE LENSES USED FOR BEAM TRANSPORT

This program determines a characteristic curve in 7-dimensional space such that any point on the curve satisfies two given matrix equations which simulate a beam transport system of quadrupole magnets.

PHY303 No Title

This program combines the pre-processing of PHY292 with PHY220, Line Shape Fitting by Variable Metric Minimization, with modifications. The result of the fitting procedure is plotted.

RE308 ANALYSIS OF STEADY MAGNETOHYDRODYNAMIC CHANNEL FLOW

This code calculates the velocity and temperature profiles, the pressure drop-flow rate gradient ratio and Nusselt number for cases of fully developed laminar flow in vertical rectangular channels.

RE313 HEAT TRANSFER IN DOUBLE PIPE HEAT EXCHANGER

The program calculates the steady state temperature distribution in a double pipe heat exchanger as a function of length and radial distance from the center. Laminar co-current flow through the exchanger is assumed.

RE321 NUCLEAR ROCKET CYCLE ANALYSIS

This is a general analysis program to evaluate steady state propellant temperatures and pressures throughout the rocket engine system at all operating conditions.

RE324 OPTIONAL GEOMETRY (AGN)

This is a utility package for calculation of pressure drop, heat transfer rates, and temperatures in systems where one-dimensional flow assumptions are applicable.

SSS145 CALCULATION OF THE DISTORTION AROUND IMPERFECTIONS IN A FACE-CENTERED CUBIC METAL

A minimization procedure is used to determine the positions of atoms in imperfect metals having a face-centered cubic crystal structure.

Listed below by title are those programs still in progress at the end of the report year:

B104	COMPUTER SERVICES REPORT FOR LABORATORY ACCOUNTING
B126	TEMPERATURE CORRECTION FOR BOMB CALORIMETRIC DATA
B127	TEMPERATURE CORRECTION FOR BOMB CALORIMETRIC DATA
B137	A MODIFICATION OF ANL-FLS, MET153 PROGRAM TO ACCOUNT FOR OVERLAPPED DATA
B141	DESIGN OF 750-KEV ACCELERATING COLUMN
B172	DEVELOPMENT OF FORMULAS FOR THE INVERSE OF THE ERROR FUNCTION
B186	A THERMAL-ELLIPSOID STEREOGRAPHIC SLIDE PROGRAM
B193	ELECTRODE POTENTIAL VS. POLARIZING CURRENT
B195	SIMULATION OF LABELED MITOSES CURVES
B196	BAND STRUCTURE CALCULATION
B197	CORRELATING FUNCTIONS FOR DISSOLUTION OF URANIUM IN CADMIUM
B199	BIG BUBBLE CHAMBER CONVECTIVE FLOW
B203	CRYSTALLOGRAPHIC CONTOUR MAPS
B204	A FIT OF CRYSTAL FIELD EQUATIONS TO MAGNETIC SUSCEPTIBILITY DATA
B205	VAPOR PRESSURE CALCULATIONS
B206	STUDY OF AUTOCORRELATION OF A STATIONARY BIRTH AND DEATH PROCESS
B207	VISCOSITY OF LIQUIDS
B209	STATISTICAL ANALYSIS OF DIFFRACTION DATA

B210 LEAST SQUARE REFINEMENT PROGRAM

B211 DETERMINATION OF CRYSTAL STRUCTURE

B212 LINEAR ENERGY TRANSFER ANALYSIS

B213 CRYSTALLOGRAPHIC PROGRAMS FOR THE 1130

B216 IRREVERSIBLE TRANSFER IN A BIMETALLIC CELL

B219 POLYCRYSTALLINE DIFFRACTION ANALYSIS

B221 CALCULATION OF EXPERIMENTAL CAPTURE CROSS SECTIONS

B222 DETERMINATION OF ISOTOPIC RATIOS WITH MULTICHANNEL ANALYSES

B226 METAL-WATER REACTIONS DURING ACCIDENT

B227 ALGEBRAIC COMPUTATIONS IN COGENT

B230 SINGLE CRYSTAL NEUTRON DIFFRACTION DATA PROCESSING

B232 PARTICLE MOVEMENT IN A SWARM OF RISING BUBBLES

B234 CONFIGURATION ENTROPY OF VACANCIES AND CATIONS IN A FLUORITE LATTICE

B235 CORROSION APPROXIMATION

B236 FIT OF RESISTIVITY VS. RADIATION DOSE

B237 NEUTRON WAVELENGTH DETERMINATION

B238 TABLES OF $Ax + Bx^2$

B239 METAL-WATER REACTION OF A FUEL ROD IN FLOWING STEAM

B240 INVESTIGATION OF THE STATISTICS OF AUTORADIOGRAPHY

C143 PHONON SCATTERING BY VACANCIES

C144 WIDTH CALCULATIONS IN METALS

C146 DIFFUSION KINETICS IV

C147 EXPERIMENTAL DATA ANALYSIS-RESISTIVITY VERSUS TEMPERATURE

C148 KINETIC ANALYSIS OF CONSECUTIVE IRREVERSIBLE SECOND-ORDER REACTIONS

C152 DECAY OF TWO INTERACTING SPECIES

C154 FOUR-PARAMETER SORTING

C155 PROTON MAGNETIC RESONANCE LINESHAPE

C157 INTERTHERMOMETER COMPARISON

C161 RESOLUTION CORRECTION

C164 DETERMINATION OF RATE CONSTANTS FOR CHEMICAL REACTIONS

C168 PARAMAGNETIC RESONANCE LINESHAPE

C170 FISSION FRAGMENT CORRELATIONS

C171 FREQUENCY FUNCTIONS OF A LIQUID

C172 ASI MULTIPARAMETER ANALYSIS

C178 TRAJECTORY CALCULATIONS FOR A MAGNETIC SPECTROMETER

C179 SPIN LATTICE RELAXATION IN MOSSBAUER SPECTRA

C180 CHARGE DISTRIBUTION IN FISSION OF U-235

C181 COMPUTATION OF SLATER-PARAMETER COEFFICIENTS, ENERGY LEVELS,
AND ATOMIC SPECTRA

C184 THERMOCOUPLE CALIBRATION PROGRAM

C185 DEBYE SPECIFIC HEAT FUNCTION

H122 MAP - SPATIAL RECONSTRUCTION OF WIDE GAP SPARK CHAMBER TRACKS

H123 PRINTAP 2

H124 INTERMEDIATE BOSON CROSS-SECTION CALCULATION

H126 GENRAT - SIMULATION OF BUBBLE CHAMBER EVENTS

H127 MAESTRO - A PROGRAM FOR THE REAL-TIME GENERATION OF MUSICAL SOUNDS

I100 DATA ACQUISITION AND/OR TIME-SHARING VIA REMOTE CONSOLE

I101 MONTE CARLO MODEL FOR 3600 OPERATIONS

I102 PERT STUDY FOR SYSTEM/ 360 ACQUISITION

I103 ZGS SPARE CABLE INDEX

I104 TOPOLOGICAL PROPERTIES OF TWO-DIMENSIONAL SELF-RESTRICTING MAZES

I106 SELECTIVE DISSEMINATION OF INFORMATION UTILITY ROUTINE

I108 COMPLETE RESPONSE CHARACTERISTICS OF GAMMA-RAYS INCIDENT ON VARIOUS
MATERIALS OF FINITE GEOMETRIES

I110 FINGERPRINT CLASSIFICATION AND IDENTIFICATION

I112 JOURNAL CHANGE PROGRAM

I113 SDI MATCHING PROGRAM

P103 CONVERSION AND REDUCTION OF RIDL CHANNEL ANALYZER DATA

P140 CALCULATIONS OF SPIN-SPIN RELAXATION IN $\text{Fe}(\text{NH}_4)(\text{SO}_4)$

P141 CYLINDRICAL CAVITY FIELD COMPUTATIONS

P142 DATA REDUCTION OF METEOROLOGICAL READINGS FOR 1949-1965.

P143 MOSSBAUER SPECTROSCOPY

P144 MOSSBAUER OPTIMIZATION

P145 ABERRATIONS OF QUADRUPOLE FOCUSING ARRAYS

P147 CHOPPER TRANSMISSION ANALYSIS

P151 ATMOS I

P152 ANALYSIS OF WIND TURBULENCE

P153 ABACUS

P154 FOUR-PARAMETER ANALYZER ANALYSIS

P156 PHYLIS LIBRARY TAPE SYSTEM

P157 64K MEMORY I/O ROUTINES FOR PHYSICS DIVISION ASI 210

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P159 ASI-210 FORTRAN I/O ROUTINES

P160 ASSEMBLER FOR THE IBM 1130

P161 ENERGY LEVELS AND WAVE FUNCTIONS OF A BOUND NUCLEON

P162 PROGRAM FOR ENERGY CALIBRATION

P163 PROGRAM FOR THE DERIVATION OF Q VALUES

P164 PROGRAM FOR THE DERIVATION OF CROSS SECTIONS

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R111 ACORN, AUTO-CORRELATION, CROSS-CORRELATION, NOISE REJECTION
R147 COUNTER-CURRENT FLOW DOUBLE PIPE HEAT EXCHANGER PROBLEM
R149 TRAFICORPORATION
R150 SYSTEMS EVALUATION
R151 UO₂ PHONON DISTRIBUTION
R152 CANDID
R154 ROCKET CYCLE ANALYSIS
R155 PRELIMINARY DESIGN OF AN INDUCTION MHD GENERATOR
R156 FOIL COUNT CALCULATIONS
R157 DOPPLER BROADENED CROSS SECTIONS
R158 EVALUATION OF HEXAGONAL FUEL ELEMENTS
R160 LIQUID FILM GENERATOR OPEN AND CLOSED CIRCUIT ANALYSIS
R161 DEFLECTION AND STRESS ANALYSIS FOR THIN PLATES AND TUBES
R163 CANDID1D
R164 MHD CYCLE EFFICIENCY ANALYSIS
R165 MISCELLANEOUS PROGRAMS (AMD PROGRAM LIBRARY)
R166 TRANSCENDENTAL BESSEL EQUATIONS ROOTS
R167 TRANSPORT DELAY SUBROUTINE
R168 COOLANT EXPULSION STUDIES - DATA REDUCTION
R169 SATURATED - COUNT RATE CALCULATION FOR ACTIVATED LIQUIDS

PROGRAMMING RESEARCH AND DEVELOPMENT

Systems Programming

A. Support Projects

Argonne's principal computation system has been the Control Data 3600 computer and its auxiliary 160-A computers, one of which is a satellite to the 3600. Continuing support for this complex has included the following projects:

1. Maintenance and modification of manufacturer-supplied programming systems.

Work has continued in the maintenance of the programming systems supplied by Control Data Corporation. As corrections and improvements are issued by the manufacturer, they are inserted into Argonne's version of the programs. The Argonne version includes extensive modifications to fit the manufacturer's generalized system to Argonne's specific needs; the most recent are detailed below.

2. SATCOPS

A support system utilizing the satellite and the disk file is scheduled for operational use in October 1966. Its major functions are the reducing of turnaround time and the increasing of throughput. Turnaround time is reduced by eliminating sequential queuing of both 3600 input and output. This is achieved by utilizing the disk file as an intermediate storage device rather than magnetic tape. Jobs are automatically scheduled for execution by the satellite 160-A and their output automatically directed to any of three printers. Throughput is increased by the scheduling of tape mounting by the satellite before the job is assigned for execution.

3. FORTRAN disk file software

Programming to support use of the disk file for FORTRAN programmers is continuing and is nearly operational. The program features two separate modes of operation: tape-like and random access. The tape-like mode allows the user to choose between use of tape and disk on the basis of operational characteristics of the application program after the application program has been written. The ability to switch easily gives the user an alternate course in case of device failure. The random access mode is designed to give the user full access to the random access capabilities of the disk.

4. Plotting subroutines

A compatibility package has been written to give the user a choice of plotting devices (either DD80 Cathode Ray Tube or Calcomp plotter) without the necessity for change in the application program. The user can choose the device on the basis of turnaround, economy, and type of recording; he need no longer consider the effort of reprogramming to effect a change.

5. Operating system instrumentation

Effort has been expended to determine the characteristics of the interaction of the operating system and the normal computation load. The principal objectives have been to measure operating system efficiency, to get a definite picture of the characteristics of Argonne's computing load and to study the effects of operating system changes on the job load. Work is virtually complete and a report will be issued shortly.

6. Peripheral support

Revision of peripheral support programs to consolidate individual functions has been initiated. The objective is better utilization of equipment and reduction of operator handling of peripheral programs and tasks.

7. Education and consultation

An increased effort has been underway to supply the users of the 3600 computer with timely aid and information. This has taken the form of assigning one person to the task as a full-time job. In addition to aiding the user, it has had the added benefit of supplying the systems programming personnel with pertinent information on incipient problems.

B. PHYLIS

The PHYLIS system consists of an ASI-2100 computer with a wide variety of peripherals located in Argonne's Physics Building and an 800-foot direct communication link to the Control Data 3600 computer. This link permits physics experimenters at either a 4.5-MEV Van de Graaff or a 12-MEV tandem Van de Graaff direct access to the Control Data 3600 on a real-time interrupt basis.

Whenever interrupts from PHYLIS are recognized, execution of the current program in the 3600 is stopped, all information needed to resume this program is preserved, and control goes to load and execute a specified PHYLIS analysis program. Later the interrupted program and the resident section of the SCOPE monitor are reloaded and control is returned to the point of interruption.

This real-time processing gives a physicist the ability to do elaborate computations quickly while his experiment is actually running. The benefits are noteworthy in that he can immediately evaluate his progress and make intelligent judgments on what further measurements he should make.

Two analysis programs are currently in use and a third is to be finished in the summer of 1966. POLARIS has been used mainly by 4.5-MEV Van de Graaff users to calculate cross sections from angular distribution data. Primarily for 4.5-MEV users also is COMBO, a program calculating differential cross sections and polarizations for neutrons of zero-spin nuclei. In final test is program Pl, a sorting and analysis program on two-parameter multi-channel analyzer data.

Numerical Methods

Recent additions to the subroutine library for the Control Data 3600 include programs for the logarithm of the real gamma function, Fresnel integrals, and Fermi-Dirac integrals. Work is in progress on routines for the elementary hyperbolic functions and the complex gamma function. Many of these routines are based on new rational Chebyshev approximations generated locally for this purpose.

In addition to the above, a routine for the solution of ordinary differential equations by either the Bulirsch-Stoer (rational extrapolation) method or the Neville (polynomial extrapolation) method has been completed in both a single and a double precision version. Extensive testing and comparison with Adams-Moulton and Runge-Kutta schemes indicates the new methods have a general advantage over the older methods both in speed for a given accuracy and in maximal accuracy attainable.

The immediate future involves reprogramming much of the subroutine library for the System/360 machines and active participation in a SICNUM*-sponsored working group to investigate testing and certification techniques for numerical subroutines.

*Special Interest Committee on Numerical Mathematics of the Association for Computing Machinery.

High-Speed Graphical Data Output Techniques

In problems where large volumes of heterogeneous output data (e.g., intermixed lines, points, and characters) must be displayed and/or photographed, conventional data formatting techniques have sometimes proved to inflict critical time penalties. Programming techniques have been developed at Argonne for use with FORTRAN to alleviate this data-formatting bottleneck for the DD80A on the Control Data 3600.

One application of these techniques has been to computer-generation of animated line-drawing motion pictures. Although this work is in a very early stage, encouraging results have been obtained thus far.

Recent Developments in Automatic Theorem-Proving

One of the undesirable side-effects encountered in using the set-of-support strategy* in computer theorem-proving is that theorems for which unit-proofs could be obtained are forced into the realm where only non-unit-proofs are obtainable. (A unit-proof is one not requiring an inference based upon two disjunctive clauses.) In order to alleviate this side effect, a class of theorem-proving strategies called extended set-of-support strategies has been formulated and is now under study. These strategies are currently being implemented on the Control Data 3600. Results obtained thus far indicate that, in addition to alleviating the side effect described above, these strategies also produce a further reduction of the set of inferences to be tested in searching for a proof of a given theorem.

Proposed General-Purpose Programming System for Non-numerical Calculations

There are many large scientific computations of great interest in which non-numerical manipulations play an important or even predominant role. For such calculations certain relatively new programming techniques, such as dynamic storage allocation with garbage collection, are very useful, sometimes essential. At the present time these techniques are implemented only in some special-purpose programming systems. Thus the programmer of such a calculation often has to choose one of three unpleasant alternatives: build his own system from scratch in assembly language, program in something like FORTRAN using less-effective, more-cumbersome techniques, or use a rigid special-purpose system with consequent inconvenience and great inefficiency.

The aim of the current research effort in this area is to improve the situation by developing a general-purpose programming system for such calculations. The system will provide comprehensive storage recovery procedures and a capability for controlling asynchronous tasks while placing only minor restrictions on the efficiency of programs and the representation of data in the computer.

*The Efficiency and Completeness of the Set-of-Support Strategy in Theorem Proving, by Lawrence Wos, George A. Robinson, and Daniel F. Carson, Jour. ACM, Vol. 12, No. 4 (October 1965) pp. 536-541.

Programs will be written in a macro-language which allows the user to re-define or extend the meaning of basic operators, introduce new operators, and write multi-argument macro-expressions in the function notation. In all parts of the program the user will be able to intermix machine language instructions and higher level expressions.

New Library Routines

ANL A950 TIØA	K. Hillstrom	3600 FORTRAN library routine for triple precision floating point input/output
ANL B155 CSIN,CCØS	K. Hillstrom	3600 FORTRAN systems routine for the complex sine and cosine
ANL C250 CUBIC	B. Garbow	Roots of cubic polynomial equations
ANL C251 QUARTIC	B. Garbow	Roots of quartic polynomial equations
ANL C252 RSSRS	W. Hafner	All roots of polynomial equations with real coefficients
ANL C358 CØULØMBF	E. Thieleker	3600 FORTRAN routine for the regular coulomb wave functions and their derivatives
ANL C359 FRMDM1H	K. Hillstrom	3600 FORTRAN library routine for the Fermi-Dirac Integral $F_{-1/2}(x)$
ANL C360 FTMDP1H	K. Hillstrom	3600 FORTRAN library routine for the Fermi-Dirac Integral $F_{+1/2}(x)$
ANL C361 FRMDP3H	K. Hillstrom	3600 FORTRAN library routine for the Fermi-Dirac Integral $F_{3/2}(x)$
ANL C362 RGAMMA	K. Hillstrom	3600 FORTRAN compatible routine for the natural logarithm of the real gamma function
ANL D250 DIFSUB	N. W. Clark	3600 FORTRAN subroutine which performs one integration step for a system of first-order ordinary differential equations
ANL D251 DIFSYS	N. W. Clark	3600 FORTRAN routine which provides input/output and control for use with ANL D250 - DIFSUB to integrate a system of first-order ordinary differential equations
ANL D252 DDFSUB	N. W. Clark	3600 FORTRAN subroutine which performs one double precision integration step for a system of first-order ordinary differential equations

ANL D253 DDFSYS	N. W. Clark	3600 FORTRAN double precision routine which provides input/output and control for use with the double precision routine ANL D252 - DDFSUB to integrate a system of first-order ordinary differential equations
ANL E150 RINTP	K. Hillstrom	3600 FORTRAN library routine for rational interpolation
ANL E151 CHEBCØEF	W. J. Cody	Chebyshev series coefficients by interpolation (double precision)
ANL E206 LSQPØL	B. Garbow	Least square polynomial fit
ANL E208	C. Chamot	Arbitrary functional fit
ANL E212	C. Chamot	A general program for the evaluation of an arbitrary function, and for the least squares determination of the coefficients of a function, linear in the coefficients, involving one or more independent variables
ANL E250 VA02A	B. Garbow	Least squares functional minimization without derivatives
ANL F152 SYMINV	B. Garbow	Symmetric matrix inversion with accompanying solution of linear equations
ANL F103 CMPINV	B. Garbow	Complex matrix inversion
ANL F202 EIGEN	B. Garbow	Eigenvalues and eigenvectors of a real symmetric matrix
ANL F204 GEIGEN	B. Garbow	Generalized eigenvalue program for symmetric matrices
ANL F250 FRANCIS	B. Garbow	Eigenvalues of real matrices
ANL F251 FRANCIS	B. Garbow	Eigenvalues of complex matrices
ANL F252 GEIGEN	B. Garbow	Generalized eigenvalue program for symmetric matrices (improved version)
ANL F402 MATINV	B. Garbow	Matrix inversion with accompanying solution of linear equations
ANL I450	M. Storm	General selective and blocked BCD card-to-tape (1401)
ANL I451 SCØPIØ	M. Storm	SCOPE input card-to-tape and output tape-to-printer (1401)

ANL J550 PLOT	G. A. Robinson R. Krupp	Provides FORTRAN- or COMPASS-coded programs the capability of plotting on the on-line Data Display Inc. Model DD80A Cathode Ray Tube Display System
ANL J952 YOLYPLØT	C. Chamot	Given sets of values (X,Y) and plotting specifications, this FORTRAN subroutine generates either a graph on 35mm film from the DD80, or a CALCOMP tape for plotting a labelled graph of Y vx. X or $\log_{10} Y$ vs. X.
ANL M101 SØRT	B. Garbow	Algebraic sort
ANL M150 CSØRT	C. Chamot	Algebraic sort
ANL Q051	M. Storm	3600 FORTRAN source deck condenser (1401)
ANL Z013	B. Garbow	Variable metric minimization
ANL Z050 UNITST1	W. J. Cody	Package to test ASINF and ACØSF
ANL Z051 UNITST2	W. J. Cody	Program to test ATANF
ANL Z052 UNITST3	W. J. Cody	Program to test SINF,CØSF
ANL Z053 UNITST4	W. J. Cody	Package to test TANF and CØTF
ANL Z054 UNITST5	W. J. Cody	Program to test SQRTF, CUBERTF
ANL Z055 UNITST6	W. J. Cody	Program to test EXPF, LØGF
ANL Z056 UNITST7	W. J. Cody	Program to test PØWRF
ANL Z057 LØCF	J. Ohde	Makes available to a FORTRAN-coded subprogram actual machine addresses of its variables
ANL Z058 UNITST8	K. Hillstrom	Package to test CABS
ANL Z059 UNITST9	K. Hillstrom	Package to test CEXP
ANL Z060 UNITST10	K. Hillstrom	Package to test CATAN
ANL Z061 UNITST11	K. Hillstrom	Package to test CLØG
ANL Z062 UNITST12	K. Hillstrom	Package to test CSQRT
ANL Z063 UNITST13	K. Hillstrom	Package to test CSIN/CCØS

ANL Z064 UNITST14	K. Hillstrom	Package to test DSQRT
ANL Z065 UNITST15	K. Hillstrom	Package to test DATAN
ANL Z066 UNITST16	K. Hillstrom	Package to test DCUBRT
ANL Z067 UNITST17	K. Hillstrom	Package to test DEXP
ANL Z068 UNITST18	K. Hillstrom	Package to test DLØG
ANL Z069 UNITST19	K. Hillstrom	Package to test DSIN/DCØS
ANL Z070 UNITST20	K. Hillstrom	Package to test TANHF

Abstracts of 3600 NEWSLETTERS

The 3600 NEWSLETTER, published at irregular intervals, contains current information and news of interest to users of the CDC 3600 and its related equipment.

3600 NEWSLETTER NO. 26

7/14/65

Announcement of cancellation of releasing SCOPE 6.0 in favor of update version 6.1.

3600 NEWSLETTER NO. 27

8/17/65

More information concerning a hardware modification (Monitor Protection feature) to the 3604 computation module of the 3600 computer system. Supplements the CDC 3600 Reference Manual (Pub. 60021300) in the form of an added appendix.

3600 NEWSLETTER NO. 28

10/29/65

Recalls pertinent procedures from earlier memos regarding the scheduling of the CDC 3600 computer and re-establishes current scheduling policies.

3600 NEWSLETTER NO. 29

11/22/65

Announces the release of an updated version of the SCOPE monitor (SCOPE 5.43). Six numerical subroutines replace their counterparts on the SCOPE library tape.

Current clock readings at various points within a job are now written on the standard output tape.

3600 NEWSLETTER NO. 30

11/15/65

Pertinent information describing the release of a new 3600 system tape (PRD 10-15).

New system versions superseding older ones include:

SCOPE 6.1
FORTRAN 5.1
COMPASS 5.1
ALGOL 1.2
SQRT 2.1

3600 NEWSLETTER NO. 31

1/28/66

System consultation services reorganization.

Recommended procedures for reporting systems bugs.

3600 NEWSLETTER NO. 32

3/17/66

Identifies release of updated 3600 System tape (PRD 10-15B).

Minor FORTRAN/COMPASS corrections made.

PHYLIS system activated and possible user effects explained.

Corrections to overlay processing are listed.

Additional SCOPE control cards, REWIND and RELEASE, available for magnetic tape.

3600 NEWSLETTER NO. 33

3/31/66

Brief writeup of the 3600 DD80/CALCOMP Compatibility Package.

3600 NEWSLETTER NO. 34

6/14/66

Introductory material for SATCOPS II.

Catalog of ANL subroutine library and COOP routines available at ANL.

NUMERICAL AND MATHEMATICAL ANALYSIS

Solution of Polynomial Equations

Each intermediate polynomial of the sequence generated during a root-squaring method has the property that its roots are the squares of those of the preceding polynomial in the sequence. The original roots are thus numerically separated and can be calculated accurately. It is necessary, however, to provide a test for determining the sign of each real root.

Now a similar process but not requiring such a test has been developed. It consists in separating the roots by a root-cubing procedure that may prove to be particularly useful for parallel arithmetic processors. A program incorporating the method is being written for the Control Data 3600.

Although of less immediate practical value, a general root power method using partitioned polynomials has also been developed. It is an extension of the root-squaring and root-cubing methods.

Optimization of Integration Procedures

One appropriate measure of the accuracy of an integration procedure for ordinary differential equations is the size of the sum of the magnitudes of the coefficients in the error term. Under reasonable assumptions about the solution and its derivatives, and using such a measure, best Runge-Kutta schemes under one or more constraints have now been developed. The constraints ensure that the accuracy will be even greater as the problem reduces to that of numerically evaluating an integral. Furthermore, the methods remain competitive in the most general case.

The developed procedures, of orders three and four, have been programmed for the Control Data 3600; they have performed as predicted on a variety of differential equations.

Integer-Preserving Elimination Methods

A new set of elimination methods to obtain accurate solutions to systems of linear equations and to calculate efficiently the accurate values of determinants and their minors has been derived. Although integer-preserving, these methods tend to have an efficiency comparable to the fastest known methods of Gaussian elimination, and are faster than any known integer-preserving elimination method. A computer program to test the procedure is being written for the Control Data 3600.

Infinite-Dimensional Representations of Lie Groups

Work is in progress on the problem of representing an abstract Lie Group by a group of unitary operators acting on a Hilbert Space. When the Lie Group in question is not compact, a situation which is of considerable importance to applications in quantum mechanics, these unitary representations have in general infinite dimension. The first part of the work consists of

generalization of certain theorems of Harish-Chandra and others, which relate the theory of algebraically irreducible representations of Lie Algebras to the theory of unitary representations of Lie Groups. It is found that under relatively weak assumptions, all algebraically irreducible representations of the real Lie Algebras are subrepresentations of representations constructed in a certain standard way. These methods have been applied to obtaining somewhat detailed results on the irreducible representations of the pseudo-orthogonal groups over the real numbers. In this case one can solve the somewhat delicate problem of finding the irreducible subrepresentations of these "standard" representations.

Hilbertian Structures

The structure theory of Krein, Moser, Gelfand, and Lidskii for stable symplectics on finite-dimensional spaces, previously used at Argonne in a mass spectrometer trajectory calculation (1504/PHY 258, July 3, 1962; coded by R. Hamelink), has been generalized to the infinite-dimensional case.

Numerical Integration on Compact Groups

As a long-term project, techniques of numerical integration on various compact groups are being collected. Recently a method based on construction of a fundamental domain in the group manifold as acted on by left and right multiplication by elements of a suitable discrete subgroup has been applied to the rotation group $O(3)$ for the purpose of disorienting certain biological organisms. Following instructions on a computer-produced tape, the organism is moved in such a way that the effects of all orientation-dependent forces on its development are, to any desired degree of accuracy, replaced by their averages over $O(3)$ with respect to Haar measure. The code and associated electronic hardware have been debugged and the biological experiment is now in progress. A mathematical description of the method will appear in a biophysical journal.

Transport and Diffusion Theory

(a) The book, Computing Methods in Reactor Physics, (Addison-Wesley) to appear in 1967, will include two chapters by members of Argonne's Applied Mathematics Division. They are: One-Dimensional Diffusion Theory (Chap. I), by M. Butler and J. Cook, and Mathematical Foundations (Chap. VIII), by J. Cook.

(b) Another book, Stochastic Transport Theory, by J. Moyal and P. J. Brockwell, is also being written.

(c) Moyal's theory of first-passage processes has now been extended by him to multiplicative processes.

COMPUTER UTILIZATION IN DIVISIONAL RESEARCH

Optics of Axially Symmetric Electron Lenses

A rather flexible system of programs has been constructed for facilitating the design of axially symmetric electron lenses. This work was done in connection with the development of the Crewe scanning electron microscope and also in support of the proposed AMU-ANL* electron microscope research facility. The inputs to the basic lens program are the electric potential function and the magnetic field magnitude along the axis of rotation of the system. Quantities computed are parameters describing the first-order optical properties and third-order aberrations of the lens. All calculations are carried out in relativistically correct fashion. The electrode surface coordinates are also computed and output onto paper tape in the proper format for input to numerically controlled machine tools.

With the aid of these programs, a 50,000-volt electron gun has been designed with an unexpectedly low spherical aberration constant of about .01 (in units of lens length).

A further elaboration of the system permits analysis of an arbitrary array of such lenses disposed along a common optic axis; in this way preliminary studies have been made of some possible accelerating tube designs for the AMU-ANL facility.

The Multiple Compton Scattering of Low Energy Gamma Radiation

The softening of low energy gamma radiation which passes through a slab of scattering material has been studied analytically by Chandrasekhar and O'Rourke. A method which seeks to improve on their approximations to the spectral intensity of transmitted radiation has now been developed and applied to derive spectral intensities for several slab thicknesses. As a check on these results a Monte Carlo program was written to trace the paths of photons scattered isotropically in a slab of finite thickness. The program gives histograms for the required spectral intensities which are in good agreement with the predicted results.

Recent Progress in Biological Image Processing

The major effort in biological image processing has been directed toward computer analysis of chromosome spread photographs. Considerable energy was expended during the past year in rewriting the previous cumbersome system of programs as a single package to run on the Control Data 3600 computer system. One phase of this has been accomplished, in that the programs for reading the CHLOE input tapes and producing the output karyograms have been rewritten and greatly improved in flexibility. However, the recognition algorithm which identifies individual chromosomes is still under study; consequently, the "training" procedures for determining recognition parameters from typical data have not yet been reprogrammed.

*Associated Midwest Universities - Argonne National Laboratory.

Another project is aimed at precise densitometry of bone autoradiographs and microradiographs. It was found feasible to modify the chromosome scanning program to cause the CHLOE machine to function as a densitometer. The most important added function is the calibration and stabilization of CRT beam intensity in terms of primary reference standards of optical density.

Convective Flow and Bubble Chamber Design

The study of convective fluid flow, both forced and free, is relevant to the design of all manner of experimental apparatus, and specifically to the design of heat exchangers and of bubble chambers.

The numerical approach made has consisted of experimenting with the techniques of Fromm et al., (LA-2910) and of Harlow et al., (LA-3425), adding modifications to deal with axisymmetric problems. To date, the Bousinesque approximation to the Navier-Stokes equation has been used to introduce convective effects. This is adequate when the scale of the problem is sufficiently small. The more complete treatments required for a body of liquid hydrogen in a bubble chamber are under development.

The on-line display facilities at Argonne have proved very valuable in the portrayal of streamline and isotherm maps. Such displays aid the programmer in his task and have enabled the bubble chamber design group at Argonne to indicate the most useful directions of program development.

Quantitative Taxonomy

A project underway seeks a quantitative measure of classifiability of attribute data from a large sample of objects. The measure should indicate whether values of one group of attributes can be used to determine another attribute by means of the classification. An attempt is being made to find statistical assumptions that would relate this problem to Shannon's coding theorems.

Biological Models

It has recently been demonstrated that mathematical models for the dynamic properties of blood-forming and -utilizing processes satisfy certain conservation laws. The usefulness of these laws lies in the fact that they are independent of most of the details of the model. The investigation brought to notice that these laws were violated by experimental results. An attempt is being made to modify the model so as to eliminate these discrepancies.

COMPUTER ENGINEERING AND COMPUTER SYSTEMS

Automatic Film Scanning

The CHLOE system has now been used as a production measuring device for over a year. Although the major component of its work has been spark chamber film produced by high energy physicists, the CHLOE equipment has shown itself to be very adaptable to a variety of applications. These applications, reviewed¹ in a recent paper, include work connected with bubble chamber film, spark chamber film, a variety of biological applications, the digitization of fingerprint patterns, and measurement of a variety of oscilloscope trace photographs. Since the time of the referenced paper, other CHLOE applications have included: digitizing smoke plume photographs (connected with atmospheric dispersion studies), studying photographs of balls flowing down pipes in order to determine flow characteristics, measuring areas and perimeters of bone cross sections, and the photographic retrieving of data from a 400-channel analyzer, fully sampled 1000 times per second.

A new and more precise scanning system called POLLY is now being constructed. Bubble chamber film will be its first major challenge. The High Energy Physics Division at Argonne is quite interested in the possibility of constructing a production version of POLLY for use in their bubble chamber film-measuring program. Their plans have been outlined in an unpublished paper.² Its main difference over the prototype, POLLY, is in the size of the control computer. It is hoped that a more powerful machine will enable the geometrical reconstruction and physical data fitting to be performed immediately on the measured data.

Analog and Hybrid Developments

The new Reeves Reac 550 analog computer delivered in November of 1965 was tested and found to be working well enough to be used for computations, although some manufacturing defects and minor design errors have been detected and subsequently repaired. This computer, because of its electronic switching, extended high-frequency response, and servo-set potentiometers, is well suited for use as the analog part of Argonne's Hybrid (analog-digital) Computing System.

This System consists of a stored-program digital computer connected through a link to two analog computers. The digital computer employed is a Digital Equipment Corporation PDP-7 with 8,192 18-bit words of core memory. The link, or Real Time Communicator (RTC), is composed of a digital control

¹Photographic Scanning Systems in the Applied Mathematics Division (ANL), D. Hodges, Seminar on Use of Computers in Analysis of Experimental Data and Control of Nuclear Facilities, May 1966, Argonne National Laboratory (in press).

²Plan for an Automatic Bubble Chamber Film Measuring System, R. J. Royston and D. Hodges, Argonne National Laboratory, July 1966 (unpublished).

unit (DCU) and an analog control unit (ACU). The analog computers, which can be slaved together and/or connected to the RTC, are two EAI 131R consoles and the two Reeves Reac 550 consoles.

The PDP-7 communicates with the DCU by an order list. Communication is from the 18-bit accumulator of the PDP-7 to the 29-bit assembly register of the DCU. Information is transferred under control of PDP-7 input/output instructions.

Initial experience with the hybrid system has proved it quite adequate. The solution of several engineering problems using hybrid computation have been reported and will be published in the literature as follows:

1. The Application of a Hybrid Computer to the Analysis of Transient Phenomena in a Fast Reactor Core, C. K. Sanathanan, J. C. Carter, L. T. Bryant, L. W. Amiot. Transactions, Vol. 9, 1, Annual Meeting American Nuclear Society (Summary), 1966.
2. A Hybrid Computer Solution of the Co-Current Flow Heat Exchanger Sturm-Liouville Problem, L. T. Bryant, L. W. Amiot, R. P. Stein, AFIPS Conference Proceedings Fall Joint Computer Conference, 1966 (in press).
3. Hybrid Computers in the Analysis of Feedback Control Systems, C. K. Sanathanan, J. C. Carter, L. T. Bryant, L. W. Amiot, AFIPS Conference Proceedings Fall Joint Computer Conference, 1966 (in press).

Measuring Table for Bubble Chamber Photographs

LAURA, a manual-type measuring table for high energy physics bubble chamber photographs, replaces the conventional wires connecting the cross-hair indicator and shaft encoder with a beam of collimated light from a helium-neon gas laser. The table provides information in the form of two angles and the fixed included side, from which the x-y coordinates are computed, presently by an ASI-210 computer. Current efforts are being concentrated in the areas of increased accuracy and increased long term repeatability. Each angle is provided by a transformer-type angular resolver, the output of which varies in phase as the mechanical angle varies. The present resolver produces sixteen electrical cycles per mechanical revolution, and accuracy of measurement has been increased to $\pm .0009''$ of arc at $60''$ from the shaft. While the relative angle from a reference point to a measured point essentially remains a constant, the actual angle read shows a moderate dependence on circuit temperature. Temperature compensation is being incorporated into the circuitry and initial indications are that long term repeatability of the actual angle will approach the shorter term accuracy. Also being incorporated is hardware which will permit the evaluation of an angular resolver exhibiting 64 electrical cycles per mechanical revolution. This resolver will theoretically increase the measurement accuracy by a factor of 4. Indications are that a small general-purpose computer will be able to accommodate four such tables, computing coordinates and performing coordinate cross-checking.

Computer-Controlled Diffraction Equipment

Several of the shorter programs for a computer(IBM 1130)-controlled diffractometer in Argonne's Metallurgy Division have now been completed, though the larger applications and data collection programs are still in the writing or debugging stage. Most of the specifications for the control monitor have been completed, but some decisions based on resident core availability have yet to be made. A scheme of transferring to the vendor-supplied monitor for utilizing the substantial software for assembly, disk packing, and utility routines has been devised and is now working. This allows a large reduction in the software effort that ordinarily would be necessary in the development of such a system. Present experience in using the system has demonstrated the value of the inexpensive disk file for bulk program and data store in small control computers and in experiments.

The feasibility of user-written FORTRAN programs operating under the control monitor is being investigated; however, it is almost certain that only assembly language programs will be allowed initially.

Several schemes for position encoding have been tried under various load and damping conditions on the stepping motors. Efforts to maintain an accuracy of .005 degrees over a large range of damping and stepping or slewing speeds have necessitated a rather rigorous treatment of this problem. Since the IBM 1130 channel has not yet been delivered, the motor control routines have not been tested, although sufficient test equipment has been built to simulate the computer for motor testing.

The fission monitor and detector amplifiers have been delivered by the Electronics Division, and other units are on order.

The Metallurgy Division has a letter of intent in for a second computer to be delivered late in 1966, based on availability of funds. It has not currently been decided whether it will be used for X-ray or neutron diffraction.

Emulsion Track Counter

Development continues on PAULETTE, an automatic device designed to count tracks made by atomic particles in a fine-grain emulsion. The emulsion, coated on a 2" by 10" plate of glass, acts as a continuous detector for particles from an accelerator. The position and density of tracks in the emulsion indicate the energy distribution of the incident particles. Typical tracks, consisting of a series of developed emulsion grains, are from 2 to 4 microns wide and approximately 100 microns long. A lens system (enlarging by a factor of 3) images the tracks, illuminated by the dark-field method, onto the photo-cathode of a commercial image dissector tube. Electrons from the photo-cathode corresponding to the incident image are accelerated toward the rear of the tube and are focused one-to-one on a resolving plane. In the resolving plane is a rectangular aperture 7 microns by 40 microns, with the long dimension lined up with the axis of the tracks. Immediately behind the aperture is a 12-stage photo-multiplier. Signals from the photomultiplier correspond to electrons from the segment of the image currently incident upon the aperture. A scan is performed by moving the entire image horizontally across the resolving aperture.

Synchronized with the horizontal scan is a high-frequency counter, the state of which at any given time is the horizontal coordinate of the scan. When the photomultiplier produces a signal of sufficient amplitude to trigger the discriminator, the state of the counter is transferred into a PDP-7 computer through the data-break channels. The electrical scan area corresponds to a rectangle that includes 64 side-by-side scans. Each scan produces a list of coordinates which is correlated with the previous list for multiple occurrences. The analysis program determines from the list if the information meets the requirements for a track and also keeps a running total of the number of tracks. After completing 64 scans, the computer directs the plate transport to move to the adjoining scan area and then reinitiates the scan procedure. Current estimates are that a plate will be counted in one to two hours as contrasted with one day to one week by human counting.

Machine Classification and Identification of Fingerprints

Research is being conducted in the area of pattern recognition in an effort to develop a system whereby fingerprints may be classified and identical prints identified by machine. It is a project that effectively utilizes CHLOE's facility for transducing pictorial information into a computer-based numerical code.

The approach taken here is to extract two types of information from within small sample areas of the fingerprint: (1) the average slope of the fingerprint ridges flowing through the area under consideration; (2) the number of ridges which end or terminate on other ridges in the sample area.

The slope information is used to form a matrix which is oriented with respect to key points in the fingerprint. This information is used for general classification. The ridge endings and bifurcations are used as secondary classification and positive identification of an unknown print.

The current status of this effort is very encouraging. Two thousand prints have been scanned by CHLOE, and their slope information extracted. This information is being used in a program on the Control Data 3600 to develop a general classification scheme. Concurrently, a program is being developed on CHLOE to extract the ridge endings. A successful solution to this problem is expected by mid-1967.

Computer-Oriented Data Acquisition and Control Systems

A major activity of the Computer Engineering Section has been in the area of consultation with experimenters in the specification, development, and implementation of computer-oriented data systems. Facilities for biology, chemistry, metallurgy, and physics have been analyzed and designed.

The basis of this work is twofold. With the large amount of digital instrumentation and several computers now within Argonne, cooperation and coordination in the methods of acquisition and formatting of data destined for central facility processing is a necessity if significant cost and turn-around problems are to be solved. Few constraints, if any, are placed on an experimenter if the acquisition or recording equipment is initially chosen or designed within the framework of present support capabilities.

Secondly, the development of computer-controlled experiments contains much of the necessary information for design of the broader Laboratory data network which is presently under investigation. In keeping with a general philosophy of designing a data network from the experiments toward the central facilities rather than vice-versa, this development work has provided much valuable insight into many of the problems encountered in such systems.

Data Collection System

A small data collection system is presently being assembled for use in conjunction with up to four Mössbauer-effect experiments in the Physics Division. Initially two experiments will be interfaced to a small, 12-bit, 2- μ sec-cycle-time general-purpose computer through the direct-memory-access channel, with provisions for adding two more.

Each experiment utilizes a detector which is moved to and from a source such that the acceleration of the detector is linear. Each cycle of the detector is divided into 400 time-windows (channels). Data collection consists of adding the number of detector pulses associated with a particular time-window to the previously accumulated total for that same window. Total accumulations for a typical experiment require that double-precision (24-bit) storage be used. This results in 800 words of core per experiment. In addition the computer will be utilized in the "through accumulator mode" to control the display on the accumulated quantities for a selected experiment. This display will be under program control, and the typewriter will be used on an interrupt basis to select the experiment to be displayed as well as display scale factors. The computer will also be utilized for data manipulation in an off-line manner.

ARGONNE CODE CENTER

The Argonne Reactor Code Center, established in 1960, is a central agency for information on nuclear physics and reactor design computer programs. The Center handles only unclassified computer codes and restricts the distribution of Naval Reactor code packages to the United States. The scope of this activity includes:

1. the collection of reactor design computer programs and their assimilation in the Center's library;
2. the reproduction and distribution of code package material for the programs in the Center's library;
3. the editing and publication of a code abstract describing each program contained in the Center's library;
4. the maintenance and distribution of ENEA Computer Programme Library programs and code package material (ENEA is the European Nuclear Energy Agency);
5. the initiation and encouragement of and assistance in the development of standards and practices, particularly in the areas of program documentation and programming practices, that will facilitate the exchange of computer programs.

The code abstracts published under category (3) are distributed to all members of the Mathematics and Computation Division of the American Nuclear Society by the Society. Argonne Reactor Code Center code package material is deposited with the ENEA Computer Programme Library for European distribution.

From the beginning of this calendar year to date, the Center has published and distributed program abstracts for 79 program additions to the library, a single revision, and 18 ENEA program abstracts. In the same time, a total of 380 requests for computer program packages and/or program reference material and documentation have been filled.

In addition, the Center, in cooperation with installation representatives, compiled and published a survey of FORTRAN II-to-FORTRAN IV conversion efforts underway in the area of reactor design and nuclear physics calculations. In conjunction with Center activity, the American Nuclear Society Mathematics and Computation Division is presently printing and distributing a proposed standard for computer program documentation and work is progressing on a collection of benchmark problems. Such a collection would be deposited in the Argonne Center library and distributed in the same manner as computer programs.

DIGITAL COMPUTER OPERATIONS

During the year 1965-1966, the Control Data 3600 and IBM 704 Computers performed the bulk of the computational assistance to Argonne's scientists and technicians.

CDC 3600

The CDC 3600, located in the Applied Mathematics Building, was operated continuously to permit the best possible service to customers with experiments under way and to others with needs for relatively fast turnaround. Turnaround during the normal day hours, Monday through Friday, varied with the length of the queue and other factors from one and one-half hours to three hours for the shorter jobs. Programming is under way to utilize equipment to better advantage and to reduce these times.

During the daytime and the early evening, jobs of less than two minutes' total duration were expedited; when no jobs of this category were available, jobs of less than ten minutes' total duration were run. Longer jobs and attended runs were completed as time permitted. During a normal Monday through Friday, 200 to 250 jobs were run between 8:30 AM and 5:00 PM; some on-line systems development work was also scheduled during these hours. An average of 100 jobs of varying lengths were completed during the remaining evening and early morning hours, along with other systems development work. Total useful production for the year was 6218 hours, or 72 percent of the available time. Unused time totaled only 715 hours, nearly all of which was experienced on weekends, early in the year. During the last months of the year, 9,000 to 10,000 jobs per month were completed, with an average running time of about four minutes.

The first standard operation using the PHYLIS interrupt system occurred in March, 1966.

The DD80A and 3692 input/output typewriter were received and installed in early 1966.

IBM 704

The IBM 704 after several years of heavy usage, was declared excess to the needs of the laboratory on June 30, 1966. Its useful production, mostly in computations for the Reactor Physics, Reactor Engineering, and Solid State Science Divisions totalled 2660 hours for the year.

IBM 1401

The IBM 1401, functioning as the input/output system for the 704, and occasionally as a backup input/output system for the 3600, handled most of the miscellaneous tape-to-card, tape-to-tape, and tape-to-printer requests daily from code centers and other individual sources. In June, 1966, it was relocated in the Applied Mathematics Building, when the 704 was turned off. With the deactivation of the Argonne-built system GUS in July, 1965, one IBM 729-II tape drive was added to the 1401 to supplement the two former drives.

CDC 160-A

In the main computer complex, the two CDC 160-A computers primarily perform input and output functions of the CDC 3600. Various software improvements were developed in an attempt to reduce the turnaround time for printed results. The principal improvement, known as SATCOPS I, utilizes the 828 disk for output from the 3600; the disk immediately becomes available to a 160-A for printing. Three printers are shared by both 160-A's, while another is connected only to the Off-line 160-A; two card readers are connected to the Off-line 160-A, and one of the two is also connected to the Satellite 160-A. Punched output is performed by the Off-line 160-A through a fast card punch installed in July, 1965 and by the IBM 1401.

Remote Station 160-A's

A microwave connection to a 160-A computer in the High Energy Physics area is tied into the Satellite 160-A; transmission of input data to the 3600 and output data from the 3600 is accomplished by means of a tape-to-tape copying routine.

The 160-A computer in the High Energy Physics Building is engaged in various relatively routine data editing and transformation problems, in addition to its transmission assignments. Some customer programming of small jobs is done also.

The 160-A computer in the Reactor Divisions Building is extremely busy with smaller programs, mostly written by and for Reactor personnel who wish to perform their own computations. There are also important duties involving active experiments in the area. Recently this computer has averaged over 100 hours per week of useful computations, including much hard copy plotting with an on-line Calcomp-type plotter.

Maintenance

Maintenance of the various computers is accomplished by six Control Data engineers permanently at Argonne, and two IBM engineers, more or less full time and supplemented by others as needs develop and the supply of engineers permits. Single shift maintenance during the normal day hours was purchased from IBM for the 704, 1401, and other IBM equipment. Double shift (16 hours daily, for five days a week) was purchased from Control Data for the 3600 and two 160-A computers in the Applied Mathematics Building computer complex, while single shift maintenance was purchased for the two remote 160-A computers. The arrangements were made following detailed studies of the relative costs and advantages of the various plans available.

Graphic Output

Graphic output equipment includes the CRT DD80 direct output from the CDC 3600 to 35-mm film and an off-line Calcomp digital plotter, plus an on-line Calcomp plotter connected to the Reactor 160-A. All three devices experienced heavy usage. The off-line Calcomp was completely saturated with a queue that occasionally exceeded 48 hours and with an average usage of 140 hours per week. Investigation of the costs and advantages of new Calcomp equipment was undertaken and additional facilities are on order.

CRT output is being encouraged by the faster development of film through use of an Eastman Kodak Recordak, which has been modified to accept the take-up reel of the CRT film camera and which can develop five feet of film per minute. Volume averages 100 feet of film per day, representing output of approximately 1,500 pictures from 5 to 10 percent of the jobs run on the 3600. It is expected that usage will continue to increase.

General.

The hardware of the CDC and IBM computers has been very reliable and subject mainly to the difficulties inherent in mechanical, if not electronic, devices. However, intensive and unrelenting attention to tape cleaning, and recertifying was found necessary to insure the best possible operations. Also, similar attention to the scheduled maintenance of the tape drives was continued, with interest turned toward the possibility of better tape drive diagnostic programs.

OPERATIONS EXPERIENCE DURING THE PERIOD JULY 1, 1965 - JUNE 30, 1966

	Hours						
	Charged & Sustaining	Setup	Un- charged	<u>Maintenance</u>		Unused	Engineer- ing
				Sched.	Unsched.		
CDC 3600	6218.3	216.7	314.6	802.7	193.2	715.0	125.1
IBM 704	2660.5	--	129.1	185.3	250.6	899.3	2.0
CDC 160-A Off-line	7418.7	--	2.4	115.9	53.8	717.8	4.33
CDC 160-A High Energy Physics	2409.9	--	31.1	103.4	35.0	280.4	1.5
CDC 160-A Reactor	3427.9	--	2.8	157.2	131.4	249.2	--

- 1a. Charged - All computing and processing of data including the development of computer programs, except as noted below. A transfer of funds is involved for all time in this category. (Research time used by the Applied Mathematics Division staff is included here.)
- 1b. Sustaining - Use of authorized AMD personnel for the following purposes: developing and testing of programming systems supporting the use of the computer, demonstrations, training, and reliability testing of hardware and software, except as noted below.
2. Setup - Time consumed in setting up tapes and equipment for a "batch" of jobs processed by the monitor system.
3. Uncharged - Computer use for reruns attributable to the malfunction of the computer, peripheral equipment, supplied or AMD-supported programming systems, or to AMD clerical or operating errors.
4. Scheduled Maintenance - Time consumed for scheduled preventive maintenance by customer engineers.
5. Unscheduled Maintenance - Time elapsed between the request for, and the completion of, corrective action required by equipment malfunction.
6. Unused - Computer time not otherwise accounted for.
7. Engineering - Time consumed for Engineering Changes, new attachments, and acceptance testing, by either ANL or computer manufacturer's personnel.

Other equipment, for which formal statistics are not maintained:

IBM 1401 - Operated 12 to 16 hours per day, 7 days per week.

Calcomp Plotter - Operated 18 to 22 hours per day, 7 days per week.

CDC 160-A (Satellited to 3600) - Used approximately same hours as the 3600.

3600 COMPUTER USE

July 1, 1965 through June 30, 1966

IBM System/360

A contract has been signed with the International Business Machines Corporation for purchase by Argonne of an IBM System/360 with model 75 and model 50 processors. The model 50 will function as a single computer from its installation at the end of July 1966 until June 1967. At that time the model 75 will be installed as the principal computing unit and the model 50 will serve as a support processor for peripheral and control functions. A full complement of primary and secondary storage, input and output equipment, and visual display units is included to give the entire system flexibility as well as computing power.

Argonne's Control Data 3600 will continue to operate as before, thus ensuring an easy transition period to the new system.

The initial computer system to be installed in the Applied Mathematics Building at the end of July 1966 will be an IBM System/360 model 50 with 256bK bytes* of core storage (2 μ sec/4 bytes), six magnetic tapes, five disk drives of 7.2 million bytes capacity each, a console typewriter, two printers, and a reader/punch. In October, core storage will be doubled to 512bK bytes. Eight character-display units with input keyboards will be attached in October and two graphic display units with light pens and input keyboards in November.

In June of 1967 the model 50 is to become a support processor to an expanded system, as follows: to the model 50 will be added two more printers, another card reader/punch, a graphic film recorder, two data cells with 400 million bytes capacity each, and a disk file of 200 million bytes capacity to replace the original five disk drives. The main computer will be a model 75 with 1024bK bytes of core storage (3/4 μ sec/8 bytes, 4-way overlap), 2 million bytes of large-capacity core storage (8 μ sec/cycle**) shared with the model 50, another disk file of 200 million bytes capacity, and a 4 million-byte high-performance drum. The model 75 will have access to the disk file and the two data cells attached to the model 50. Simultaneously, any two of the original six tapes may be used by the model 75 or one each by the 50 and the 75.

*256bK = 256 times 1024 bytes; a byte is 8 binary digits.

**A cycle is 4 bytes in the model 50 and 8 bytes in the model 75.

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Demonstrate Techniques in Computer Animated Line Drawings, by George A. Robinson. Motion picture film which will be reduced to 16 mm to demonstrate techniques in computer animated line drawings; will be shown to Committee on Educational Media, American Mathematical Society, Calculus project.

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- (1) Biological & Medical Research Division
- (2) University of Ljubljana, Yugoslavia
- (3) Solid State Science Division
- (4) Illinois Institute of Technology
- (5) Michigan State University
- (6) The University of Chicago
- (7) Physics Division
- (8) High Energy Physics Division
- (9) Reactor Physics Division
- (10) Northwestern University

Argonne Reports

- 1) ANL-6987, RSSR ROUTINE - A Root-Squaring and Subresultant Procedure for Finding Zeros of Real Polynomials, by Erwin H. Bareiss and Ronald Hamelink(1).
- 2) ANL-7023, The Argonne-Revised THERMOS CODE, by B. Toppel(2) and I. Baksys.
- 3) ANL-7065, Notes on Axioms for Quantum Mechanics, by M. D. MacLaren.
- 4) ANL-7109, A Checker Playing Program for the IPL-VC Computer, by W. R. Cowell and M. C. Reed(3).
- 5) ANL-7112, XLIBIT: ANL Cross-section Library Code, by S. D. Sparck (in press).
- 6) ANL-7121, A Cathode-Ray-Tube Plotting System for the CONTROL DATA 3600 Computer, by G. A. Robinson and R. F. Krupp.
- 7) ANL-7126, The Numerical Integration of Ordinary Differential Equations of Various Orders, by C. W. Gear.
- 8) ANL-7129, Applied Mathematics Division Summary Report, July 1, 1964 through June 30, 1965, R. F. King, Editor.
- 9) ANL-7147, Modulated Reciprocal Crystal-Lattice and Diffractometric Computer Program, by M. Atoji(4) and J. Gvildys.
- 10) ANL-7149, GYRO II, A Macro-defined System for List Processing, by Daniel F. Carson and George A. Robinson (in press).
- 11) ANL-7165, Tables for the Calculation of Operating Parameters for Compound Solvent-Extraction Columns, by Terry R. Johnson(5) and Nelda K. Clark.
- 12) ANL-7194, General Input Specifications for ANL Reactor Programs, by M. Butler and H. Greenspan (in press).
- 13) ANL-7200, Rational Chebyshev Approximations for Fermi-Dirac Integrals of Orders $-1/2$, $1/2$, and $3/2$, by W. J. Cody and Henry C. Thacher, Jr.(2) (in press).
- 14) ANL-7213, Multistep Integer-preserving Gaussian Elimination, by Erwin H. Bareiss (in press).
- 15) ANL-7216, Conjugacy to Unitary Groups within the Infinite-Dimensional Symplectic Group, by Irving E. Segal(6) (in press).
- 16) ANL-7221, SNARG-1D, A One-Dimensional Discrete Ordinate Transport Theory Program for the CDC-3600, by G. Duffy, H. Greenspan, S. Sparck, J. Zapatka, and M. Butler (in press).

- 17) ANL-7231, Fortran Subroutines for Householder's Method in the Complex Case and Eigensystems of Hermitian Matrices, by Dennis J. Mueller(7) (in press).

- (1) Michigan State University
- (2) Reactor Physics Division
- (3) Stanford University
- (4) Chemistry Division
- (5) Chemical Engineering Division
- (6) Consultant; Massachusetts Institute of Technology
- (7) Resident Research Associate; Yale University

Applied Mathematics Division Technical Memoranda

- 1) No. 53, Local Optimization of CDC 3600 FORTRAN Generated Codes, by Daniel Carson.
- 2) No. 90, Conservation Laws in the Equations of Population Dynamics as Applied to the Tagging of White Blood Cells by Tritiated Thymidine, by R. Buchal, D. Phillips, M. Maloney(1), and E. Trucco(2).
- 3) No. 95, ANL-CDC Reprogramming Series IV, SNARG-1D, by M. K. Butler, G. Duffy, H. Greenspan, E. Mueller(3), S. Sparck, and J. Zapatka.
- 4) No. 102, C7A: An Assembly Program for the PDP-7 Computer Executed on a CDC-3600, by R. Clark and D. Hodges.
- 5) No. 106, MAESTRO - A Program for the Real-Time Generation of Musical Sounds, by Robert K. Clark.
- 6) No. 107, Magnetostrictive Wire Acoustic Delay Line Experiments, by V. Tantillo and B. Shelman.
- 7) No. 108, Spark Reconstruction in the CERN Film, by Robert Clark.
- 8) No. 109, Generating Functions of Confluent Hypergeometric Functions, by E. Thieleker.
- 9) No. 110, Uniform Plex Structures and the Computer Processing of Undirected Graphs, by Robert K. Clark.
- 10) No. 111, A Proposal for a Fingerprint Classification and Identification System, by C. B. Shelman. ✓
- 11) No. 112, High Energy Physics Code Abstracts, by R. J. Royston.
- 12) No. 113, Internal Sorting by Radix Plus Sifting, by M. Donald MacLaren.
- 13) No. 114, THE ROOT CUBING PROCESS, A Method for Finding the Zeros of Polynomials on Present Day and Future Generation Computers, by Erwin H. Bareiss.
- 14) No. 115, The Argonne Hybrid Computer Maintenance Manual, by L. Amiot, R. Aschenbrenner, K. Bish, and J. Byram.
- 15) No. 116, Manual for the Digital Filter, by Charles H. Conley.
- 16) No. 117, Report on the Feasibility of 3600 FORTRAN/360 Reprogramming Using the COGENT Programming System, by Leon Shalla.
- 17) No. 119, Specifications for Input/Output Drivers for the SCOPE Monitor on the CONTROL DATA 3600, by Ronald F. Krupp.

(1)Laboratory of Radiobiology, San Francisco Medical Center

(2)Biological and Medical Research Division

(3)Control Data Corporation

Papers Presented at Meetings

- 1) Banach Algebras and Asymptotic Mechanics, by J. M. Cook, Institute D'Etudes Scientifiques de Cargese, Ecole D'Ete 1965, Corsica, July 9, 1965.
- 2) The Sequential Compound Decision Problem with $m \times n$ Loss Matrix, by J. Van Ryzin, Institute of Mathematical Statistics Western Regional Meeting, Berkeley, California, July 19-21, 1965.
- 3) Uniform Convergence of Losses in the Fixed and Sequential $m \times n$ Compound Decision Problem (by title), by J. Van Ryzin, Institute of Mathematical Statistics Western Regional Meeting, Berkeley, California, July 19-21, 1965.
- 4) An Introduction to the COGENT Programming System, by John C. Reynolds, 20th National Association for Computing Machinery Conference, Cleveland, Ohio, August 24-26, 1965.
- 5) Non-parametric Bayesian Decision Procedures for (Pattern) Classification with Stochastic Learning, by J. Van Ryzin, 4th Prague Conference on Information Theory, Statistical Decision Functions and Random Processes, Prague, Czechoslovakia, September 1-11, 1965.
- 6) MAESTRO - A Program for the Real-Time Generation of Musical Sounds, by Robert K. Clark, Audio Engineering Society, New York, October 11, 1965.
- 7) Uniform Plex Structures and the Computer Processing of Undirected Graphs, by Robert K. Clark, Annual Conference on Programming for Flying Spot Devices, Columbia University, New York, October 27-29, 1965.
- 8) Inversion of Overlap Matrices for Very Long Ranges in Solids, by J. R. Gabriel and T. Arai(1), Chicago American Physical Society Meeting, October 28-29, 1965.
- 9) Shifts in the ESR Spectral Parameters of Atomic Hydrogen and Deuterium Trapped in Frozen Acids, by S. A. Marshall(1), J. R. Gabriel, and R. A. Serway(2), Chicago American Physical Society Meeting, October 28-29, 1965.
- 10) Automating Photographic Source Data from Scientific Experiments, by M. Butler, International Systems Meeting, Palmer House, Chicago, Illinois, November 1-3, 1965.
- 11) Application of Computers for Pairing Chromosomes, by A. Stroud(3), J. Butler, and M. Butler, 4th Mammalian Cytology and Somatic Cell Genetics Conference, Williamsburg Inn, Williamsburg, Virginia, November 2-4, 1965.
- 12) CHLOE: An Automatic Film Scanning Equipment, by D. Hodges, IEEE Computer Group Meeting, Argonne National Laboratory, November 18, 1965.

- 13) A Compact, Linked-List Queuing Procedure, by D. Jacobsohn, IEEE Computer Group Meeting, Argonne National Laboratory, November 18, 1965.
- 14) Experiment in Parallel Processing for Digital Perceptron Simulation, by D. Jacobsohn, Chapter Session, Professional Group on Electronic Computers, IEEE, Houston, Texas, January 20, 1966.
- 15) Computer Simulation of Percent Labeled Mitoses Curve, by G. M. Kollmorgen(3), M. D. MacLaren, and E. Trucco(3), Biophysical Society Meeting, Boston, Massachusetts, February 23-25, 1966.
- 16) Digital Processing of Biological Patterns - CHLOE, by Margaret K. Butler, Operation Interface, Argonne National Laboratory, March 16, 1966.
- 17) The Chemical Binding Effects on the Resonance Line Shapes of Uranium-238 in a UO_2 Lattice (by title), by C. R. Adkins(4), P. J. Persiani(4), R. N. Hwang(4), and J. J. Kaganove, Conference on Neutron Cross Section Technology, Washington, D.C., March 22-24, 1966.
- 18) Bayes Risk Consistency of Classification Procedures Using Density Estimation, by J. Van Ryzin, Institute of Mathematical Statistics Central Regional Meeting, Lafayette, Indiana, March 23-25, 1966.
- 19) Topological Calculations by Machine, by M. D. MacLaren and M. E. Mahowald(5), American Mathematical Society Symposium on Mathematical Aspects of Computer Science, New York City, April 5-7, 1966.
- 20) Computer Controlled Diffractometer Equipment, by R. Aschenbrenner, Seminar on Use of Computers in Analysis of Experimental Data and Control of Nuclear Facilities, Argonne National Laboratory, May 4-6, 1966.
- 21) Laser Activated Ultra-precision Ranging Apparatus (LAURA), by Robert H. Vonderohe and John H. Doede(6), Seminar on Use of Computers in Analysis of Experimental Data and Control of Nuclear Facilities, Argonne National Laboratory, May 4-6, 1966.
- 22) Photographic Scanning Systems in the Applied Mathematics Division, by D. Hodges, Seminar on Use of Computers in Analysis of Experimental Data and Control of Nuclear Facilities, Argonne National Laboratory, May 4-6, 1966.
- 23) The Application of a Hybrid Computer to the Analysis of Transient Phenomena in a Fast Reactor Core, by C. K. Sanathanan(4), J. C. Carter(4), L. T. Bryant, and L. W. Amiot, American Nuclear Society, 12th Annual Meeting, Denver, Colorado, June 20-23, 1966.

- (1) Solid State Science Division
- (2) Illinois Institute of Technology
- (3) Biological and Medical Research Division
- (4) Reactor Physics Division
- (5) Northwestern University
- (6) High Energy Physics Division

SEMINARS AND SYMPOSIA

Applied Mathematics Division Seminars

- July 8, 1965 An Introduction to the COGENT Programming System, by Dr. John Reynolds, Applied Mathematics Division, Argonne National Laboratory.
- July 22, 1965 Uniform Convergence of Matrix Powers, by Prof. Beresford Parlett, Applied Mathematics Division, Argonne National Laboratory.
- August 5, 1965 Nordsieck Revisited — The Numerical Integration of Ordinary Differential Equations, by Prof. C. W. Gear, Applied Mathematics Division, Argonne National Laboratory and University of Illinois, Urbana, Illinois.
- August 17, 1965 An Unusual Example of Numerical Instability, by Prof. Walter Gautschi, Applied Mathematics Division, Argonne National Laboratory and Purdue University, Lafayette, Indiana.
- August 17, 1965 Joint Applied Mathematics and Theoretical Physics Seminar - Theory of Twisted Convolutions and the C* - Algebras of a Free Boson Field, by Prof. Daniel Kastler, University of Marseille, Marseille, France.
- August 17, 1965 Plans for Multiple Access Organization of the Canberra 3600, by Mr. Trevor Pearcey, Commonwealth Scientific and Industrial Research Organization, Canberra, Australia.
- August 19, 1965 Calculating Orthogonal Eigenvectors of Hermitian Matrices, by Prof. William M. Kahan, University of Toronto, Toronto, Ont., Canada.
- August 24, 1965 Joint Applied Mathematics and Theoretical Physics Seminar - Aspects of the Phase Space Representation of Quantum Theory, by Prof. Daniel Kastler, University of Marseille, Marseille, France.
- August 27, 1965 Computer Control of Data Collection in Diffraction Experiments, by Prof. O. S. Mills, The University of Manchester, Manchester, England.
- August 31, 1965 Joint Applied Mathematics and Theoretical Physics Seminar - Phase Space Representation of Quantum Theory, by Prof. Daniel Kastler, University of Marseille, Marseille, France.
- September 2, 1965 On the Computation of Coulomb Wave Functions, by Professor Walter Gautschi, Applied Mathematics Division, Argonne National Laboratory, and Purdue University, Lafayette, Indiana.

- September 16, 1965 Joint Applied Mathematics and Metallurgy Seminar - The Oak Ridge Computer-Controlled X-Ray Diffractometer, by Mr. W. R. Busing, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- September 30, 1965 Approximate Solution of Functional Equations, by Dr. Victor Pereyra, U.S. Army Math. Research Center, University of Wisconsin, Madison, Wisconsin.
- October 7, 1965 Joint Applied Mathematics and Theoretical Physics Seminar - Conditional Expectations and Quantum Mechanical Measurement Theory, by Dr. James Pool, The Scientific Laboratory, Ford Motor Company, Dearborn, Michigan.
- October 8, 1965 Joint Applied Mathematics and Theoretical Physics Seminar - The Vacuum State in Field Theory, by Prof. H. J. Borchers, Institute des Hautes Etudes, Scientifiques at Bures-sur-Yvette, France, at present a visitor at the Palmer Physical Laboratory, Princeton University, Princeton, New Jersey.
- October 14, 1965 Extrapolation of Nucleon Form Factors: Pathologies of Rational Function Fitting, by Dr. F. Chilton, High Energy Physics Division, Argonne National Laboratory.
- October 15, 1965 Quasi Reversibility Methods, by Dr. J. L. Lions, Professor of Mathematics, University of Paris, France.
- October 28, 1965 Imagery by Wavefront Reconstruction, by Prof. Emmett N. Leith, Institute of Science and Technology, University of Michigan, Ann Arbor, Michigan.
- November 4, 1965 Advances in Problems in High Speed Computing Systems, by Dr. M. J. Flynn, Associate Professor of Systems Engineering, University of Illinois, Chicago Circle Campus.
- November 11, 1965 Digital Simulation by the Modified Z-Transformation Method, by Dr. James W. Daniel, IBM Corporation, Palo Alto, California.
- November 24, 1965 Difficulties in Computing Matrix Eigenvalues and How to Resolve Them, by Prof. Beresford Parlett, University of California at Berkeley, California.
- December 2, 1965 Spectral Analysis of Line Processes, by Prof. M. S. Bartlett, Visiting Professor, Department of Statistics, The University of Chicago, and Professor of Mathematical Statistics, University College, London, England.

- December 9, 1965 Search Strategies and Evaluation Problems in Automatic Information Retrieval Systems, by Prof. Gerard Salton, Department of Computer Science, Cornell University, Ithaca, New York.
- December 15, 1965 Numerical Methods for Hydrodynamic Stability Problems, by Dr. M. R. Osborne, Edinburgh University, Edinburgh, Scotland, and Computer Laboratory, Australian National University, Canberra, Australia.
- December 16, 1965 One-pass Analysis of a New Class of Unambiguous BNF Grammars, by Mr. William McKeeman, Computation Center, Stanford University, Stanford California.
- January 6, 1966 Some Stochastic Problems in the Theory of Multiple Scattering, by Mr. Peter Brockwell, Applied Mathematics Division, Argonne National Laboratory.
- January 13, 1966 Joint Applied Mathematics and Theoretical Physics Seminar - Canonical Quantization, by Prof. R. Streater, Massachusetts Institute of Technology, Cambridge, Massachusetts.
- January 14, 1966 Joint Applied Mathematics and Theoretical Physics Seminar - Spontaneous Symmetry Breakdown, by Prof. R. Streater, Massachusetts Institute of Technology, Cambridge, Massachusetts.
- January 19, 1966 Approximate Solution of Differential Equations in Chebyshev Interpolations, by Dr. John Mason, Research Associate, Institute of Fluid Dynamics, University of Maryland, College Park, Maryland.
- February 3, 1966 Banach Algebras and Asymptotic Mechanics, by Dr. Joseph M. Cook, Applied Mathematics Division, Argonne National Laboratory.
- February 10, 1966 What Models of Calcium Metabolism Can Explain Power Function Retention of Bone-Seeking Radioisotopes? by Dr. John Marshall, Radiological Physics Division, Argonne National Laboratory.
- February 17, 1966 Compilation of Syntax Analyzers in COGENT, by Dr. John C. Reynolds, Applied Mathematics Division, Argonne National Laboratory (at present on leave to Computer Science Department, Stanford University, Stanford, California).
- February 18, 1966 Double Sweep Method for Matrix Inversion, by Prof. Thomas I. Seidman, Department of Mathematics, Wayne State University, Detroit, Michigan.

- February 24, 1966 The Solution of Non-linear Boundary Value Transport Problems in Electron and Plasma Devices, by Prof. R. J. Lomax, Electron Physics Laboratory, The University of Michigan, Ann Arbor, Michigan.
- March 1, 1966 A General-Purpose Macrogenerator, by Prof. Christopher Strachey, Project MAC, Massachusetts Institute of Technology, Cambridge, Massachusetts.
- March 4, 1966 Two Quantum Field Theory Models in Two Dimensions, by Mr. Daniel Dubin, Department of Physics, New York University, New York, New York.
- March 10, 1966 Algorithms of Romberg Type with Applications to Ordinary Differential Equations, by Dr. W. B. Gragg, Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- March 24, 1966 The ILLIAC IV Program at the University of Illinois, by Prof. D. L. Slotnick, Department of Computer Science, University of Illinois, Urbana, Illinois.
- March 31, 1966 A System of Non-linear Integrodifferential Equations Occurring in Reactor Dynamics, by Prof. Jacob Levin, Department of Mathematics, The University of Wisconsin, Madison, Wisconsin.
- April 21, 1966 Lipschitz Conditions and Integrability for Characteristic Functions, by Prof. Ralph P. Boas, Chairman Mathematics Department, Northwestern University, Evanston, Illinois.
- May 16, 1966 Error Estimation in the Numerical Integration of Strongly Stable Systems of Differential Equations, by Prof. Germund Dahlquist, Royal Institute of Technology, Stockholm, Sweden.
- May 19, 1966 ILLIAC III Computer for Visual Data Processing, by Prof. Bruce McCormick, Department of Computer Science, University of Illinois, Urbana, Illinois.
- May 26, 1966 Music 4F -- A FORTRAN Music-Generating Program, by Dr. Arthur Roberts, High Energy Physics Division, Argonne National Laboratory.
- May 26, 1966 Calculation of Distribution of Number of Cells in a Growing Clone, by Dr. C. W. Gilbert, Patterson Laboratories, Christie Hospital & Holt Radium Institute, Manchester, England.

- June 9, 1966 Commutators of Matrices, by Dr. Olga Taussky Todd, Department of Mathematics, California Institute of Technology, Pasadena, California.
- June 9, 1966 Computer Insights into the Shape of Certain Four-Dimensional Regions, by Prof. Harvey Cohn, Head, Department of Mathematics, University of Arizona, Tucson, Arizona.
- June 28, 1966 Linear Threshold Devices and Perceptrons, by Prof. T. M. Cover, Department of Electrical Engineering, Stanford University, Stanford, California.
- June 30, 1966 The Analytic Continuation of the Resolvent Kernel and Scattering Operator Associated with the Schroedinger Operator, by Prof. C. L. Dolph, Department of Mathematics, University of Michigan, Ann Arbor, Michigan.

Applied Mathematics Division Summer Meetings, September 7-10, 1965

Participants in the Conference on Numerical Methods for Solving Partial Differential Equations were (in addition to several from Argonne):

G. Birkhoff	B. Parlett
J. M. Gary	S. Parter
R. B. Kellogg	R. S. Varga
H. O. Kreiss	C. H. Wilcox
M. Lees	D. Young

Applied Mathematics Division Special Interest Seminars

- March 3, 1966 Numerical Solution of One-Dimensional Reactor Kinetics Equations (A Reactor Physics Seminar), by Dr. Kent Hansen, Nuclear Science and Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts.
- March 9, 1966 Experiences with the CDC 6600 at CERN, by Mr. Richard Royston, Applied Mathematics Division, Argonne National Laboratory. On assignment to CERN from October 1965 to October 1966.
- March 17, 1966 Reactor Noise, by Mr. Harold Greenspan, Applied Mathematics Division, Argonne National Laboratory.
- June 23, 1966 Finite Memory Two-Armed-Bandit Problem, by Mr. Daniel Gans, Department of Mathematics, University of Illinois, Urbana, Illinois.

Conference on Finite Difference Methods for Solving Partial Differential Equations

A small conference on this topic was held in the Applied Mathematics Division during the week of June 20-24, 1966. It was the fifth in a series of annual meetings on this topic sponsored by Argonne. The participants in the conference are Argonne staff members and visitors who are specialists on finite difference methods and related subjects. The visitors at this year's conference were G. Birkhoff (Harvard University), J. H. Bramble (University of Maryland), P. Ciarlet (Case Institute of Technology), B. E. Hubbard (University of Maryland), M. Lees (Case Institute of Technology), B. Parlett (University of California, Berkeley), R. Richtmyer (University of Colorado), M. H. Schultz (Case Institute of Technology), R. S. Varga (Case Institute of Technology), O. Widlund (University of Upsala), J. H. Wilkinson (National Physical Laboratory), and D. Young (University of Texas).

The conferences are informal, consisting of consultation on problems of mutual interest among Argonne staff members and visitors, and a series of talks. This year the speakers were: G. Birkhoff, J. H. Bramble (on joint work with B. E. Hubbard), P. Ciarlet (on joint work with R. S. Varga), R. Richtmyer, M. H. Schultz (on joint work with M. Lees), O. Widlund, David B. Taylor (Argonne), and C. H. Wilcox (Argonne).

Participants are chosen because of their common interests in one or more areas of finite difference theory. The conferences have been effective in advancing research on methods for the numerical solution of partial differential equations by producing intensive discussions which have led to new ideas and results.

Study Seminars

A weekly seminar lecture series entitled Transport Theory and Stochastic Processes, with Dr. J. E. Moyal of the Applied Mathematics Division in charge, started on March 23, 1966.

Mathematical Methods of Quantum Theory,

a working seminar series conducted by Dr. J. E. Moyal, started on March 29, 1966. Seminars have been given by Dr. J. C. T. Pool of the Applied Mathematics Division, Argonne; Dr. Hans Ekstein of the Physics Division, Argonne; Mr. James Wray of Syracuse University; and Mr. Ernest Thieleker of the Applied Mathematics Division, Argonne.

University and Symposium Presentations

Integrated Circuit Technology, by R. Aschenbrenner, Jodavpur University, Calcutta, India, March 1965.

Future Trends in Circuit Integration for Computers, by R. Aschenbrenner, Institute of Electrical Engineers, Calcutta, India, May 1965.

Evaluation and Revolution in Digital Computer Design, by R. Aschenbrenner, Central Engineering Research Institute, Pilani, India, May 1965.

The Computer's Role at Argonne, by Margaret K. Butler, NSF Summer Institute, Bradley University, Peoria, Illinois, August 5, 1965.

Theorem Proving with Computers, by L. Wos, Stanford University, Palo Alto, California, September 1965.

Introduction to the COGENT Programming System, by John Reynolds, Computer Science Department Colloquium, Stanford University, Stanford, California, October 18, 1965.

Some Applications of Computers in Engineering and Science, by J. W. Butler, Young Engineers Forum (Western Society of Engineers), Engineers Club, Chicago, Illinois, November 10, 1965.

Scientific Applications, Data Processing 101; Margaret K. Butler, participant, Television Channel 11, City of Chicago Junior Colleges, November 1965.

An Introduction to the COGENT Programming Language, by John Reynolds, Applications Seminar, Development Division, Control Data Corporation, Palo Alto, California, November 11, 1965.

Machine Computation of a Spectral Sequence, by M. D. MacLaren, Stanford Computer Science Colloquium, Stanford University, Stanford, California, November 1965.

Continuous Transformations and Stochastic Differential Equations, by D. Woodward, Mathematics Colloquium, Northern Illinois University, DeKalb, Illinois, January 11, 1966.

Non-parametric Bayesian Decision Procedures for (Pattern) Classification with Stochastic Learning, by J. Van Ryzin, Ohio State University, Columbus, Ohio, February 8, 1966.

Decision Theoretic Approach to Pattern Recognition, by J. Van Ryzin, Wayne State University, Detroit, Michigan, February 9, 1966.

An Introduction to the COGENT Programming System, by John Reynolds, Computer Sciences Department Colloquium, Purdue University, Lafayette, Indiana, February 14, 1966.

Syntax Analysis in COGENT, by John Reynolds, Guest Lecture in course on Programming Systems, taught by Prof. Saul Rosen, Purdue University, Lafayette, Indiana, February 14, 1966.

An Introduction to the COGENT Programming System, by John Reynolds, Computer Sciences Department Colloquium, University of Wisconsin, Madison, Wisconsin, February 15, 1966.

Syntax Analysis in COGENT, by John Reynolds, Computer Sciences Department Seminar, University of Wisconsin, Madison, Wisconsin, February 16, 1966.

Multiplicative Processes in Physics, by J. Moyal, University of Arizona, Tucson, Arizona, February 16-25, 1966.

A Proposal for a Fingerprint Classification and Identification System, by C. B. Shelman, Cook County Medical Center, Chicago, Illinois, February 21, 1966.

First Passage Distributions in Transport and Multiplicative Processes, by J. Moyal, University of Arizona, Tucson, Arizona, February 16-25, 1966.

Syntax Analysis in the COGENT Programming System, by John Reynolds, Computer Science Department Seminar, Stanford University, Stanford, California, February 23, 1966.

Trends in the Development of the Curriculum in the Mathematical Sciences, by W. Givens, Symposium on "The Recommended Impact of Computer Applications on the Undergraduate Mathematics Curriculum," Florida State University, Tallahassee, Florida, March 14, 1966.

Repetitive Statistical Decision Processes, by John Van Ryzin, Colloquium Series, Marquette University, Milwaukee, Wisconsin, March 17-18, 1966.

On the Probability Problem of Pattern Classification Learning Algorithms, by J. Van Ryzin, Seminar at Information Processing and Control Systems Laboratory, Northwestern University, Evanston, Illinois, April 14, 1966.