Abstracts of Computer Programs and Data Libraries Pertaining to Photon Production Data

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ABSTRACTS OF COMPUTER PROGRAMS
AND DATA LIBRARIES PERTAINING TO
PHOTON PRODUCTION DATA

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ABSTRACT

Abstracts, or descriptions, of computer programs and data libraries pertaining to Photon Production Data (Measurements, Evaluations and Calculations) maintained in the collections of the Radiation Safety Information Computational Center, Oak Ridge, Tennessee USA and at the OECD/NEA Data Bank, Paris, are collected in this document.
SECTION 1
INTRODUCTION

In 1994 the International Atomic Energy Agency authorized a Coordinated Research Programme (CRP) for the purpose of addressing open problems in photon production, focusing on neutron-induced reactions in the standard energy range. Two meetings of the CRP have been held: the first in November 1994 held in Bologna, Italy; the second in May 1996 held in Vienna. One of the goals of the CRP was to provide methods for handling photon data, and it was considered important to provide a list of existing codes available in the documentation centers. At the second CRP meeting the following Action was placed on one of us (Dickens; USA): "A tabulation will be made of general codes important for photon production currently available at the Radiation Safety Information Computational Center at ORNL, Oak Ridge, and at OECD/NEA Data Bank, Paris. This should be supplemented by comments and assessments of the codes."

This document contains abstracts or descriptions of 50 codes and 8 photon data libraries available from the respective specialized information analysis centers. These 50 codes are separated into four categories, namely experimental data reduction by (a) photon peak analysis, or by (b) unfolding; (c) model predictions; and (d) miscellaneous. A fifth category presents information on the data libraries.
SECTION 2
PEAK ANALYSIS CODES

These are programs designed to analyze gamma-ray spectra obtained with high-resolution Ge or Si detectors. A program identifies peaks in the spectrum, determines the net yield in counts in a given peak, and then, depending upon the design of the code identifies the centroid of the peak with a photon energy and the yield with the number of detected photons. The computer codes use different methods for defining peaks, backgrounds, identifications, and (when included in the program) determination of the responsible radionuclide(s).

Comments and assessments: the computer codes are written by scientists usually to accommodate a research activity, an activity which may involve a specific computer environment and/or a specific programming language. This observation is one reason that the compilers do not make a recommendation for choice of code to use. The second reason relates to a study done by Parr, Houtermans, and Schaerf who, in 1978, did a study involving 47 users of 4 different codes; the major conclusion of these authors was:

"Perhaps rather surprisingly each of these four programs produced results covering a wide range of performance, demonstrating once again that it is the user rather than the program who plays the major role in determining the quality of the results."

Two of the tested codes, GAMANL and SAMPO, have since been improved and are included in the present compilation. However, the compilers suggest that the above conclusion remains valid for all but rote applications; certainly for fundamental studies user interpretation of computer-program results is a necessity.

REFERENCE

1. NAME AND TITLE
   **ACTIVE-PC**: A Program to Process Gamma or X-ray spectra.

2. CONTRIBUTOR
   Joint Institute of Nuclear Research, Dubna, USSR, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; all IBM PC's.

4. NATURE OF PROBLEM SOLVED
   ACTIV analyzes gamma-ray spectra measured by various types of detectors and under a large variety of conditions.

5. METHOD OF SOLUTION
   ACTIV performs calibration of the measurement apparatus. It deletes outliers from the spectrum. It also creates peak models with the use of histograms. The spectrum is divided into several intervals and peak search is performed in each of these intervals. A least squares estimator is used to determine peak positions and areas.

6. RESTRICTIONS OR LIMITATIONS
   A maximum of 20 peaks in the spectrum interval can be handled.

7. TYPICAL RUNNING TIME
   At the NEA Data Bank, the sample problem took about 343 seconds on an IBM PC/AT with a math co-processor. At RSICC, the same problem took about 590 seconds on an IBM PC/XT with a math co-processor; compilation of all Fortran sources took about 60 minutes and linking took 12 minutes.

8. COMPUTER HARDWARE REQUIREMENTS
   IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code was written in Fortran 77 and uses RM Fortran Version 4.0 or higher compiler. The PLINK86 overlay linker is also necessary.

10. REFERENCE
    "The Long Write Up of the Program ACTIV," informal notes by V. B. Zlokazov, JINR, Dubna, USSR.

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and one DS/DD (360 K) 5.25 inch diskette.

12. DATE OF ABSTRACT
    November 1990.
KEYWORDS: MICROCOMPUTER; GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE
1. **NAME AND TITLE**

   **AMUSE**: Gamma-Ray Spectra Unfolding Code.

2. **CONTRIBUTOR**

   Los Alamos National Laboratory, Los Alamos, New Mexico.

3. **CODING LANGUAGE AND COMPUTER**

   Fortran 63; CDC-6600.

4. **NATURE OF PROBLEM SOLVED**

   AMUSE unfolds complex gamma-ray spectra obtained with Ge(Li) detectors. It will analyze 20 independent regions in a spectrum with up to 350 data points and 11 full-energy lines in each region. Gaussian and exponential functions represent the data analytically. The best least-squares values of the energy, area, and width can be obtained for each full-energy peak.

5. **METHOD OF SOLUTION**

   AMUSE determines the number of counts in the full-energy peaks of complex gamma-ray spectra. A sequence of related spectra is recorded on magnetic tape, along with identification information. For unfolding, the first spectrum in the series is divided into regions that contain the peaks to be analyzed. Estimates of certain parameters are made and then each region is analyzed separately. If subsequent spectra use the same regional divisions, it is possible to use the results of one spectrum as the estimates for parameters in the following spectrum.

   A Gaussian function with two exponential tails on its low-energy side is fitted to each full-energy peak. A single exponential function is then fitted to the entire region to represent contributions from higher-energy lines and background. The sign and magnitude of each parameter are checked after each iteration to prevent the least-squares analysis from diverging.

   Spectra are taken in sequence from different positions on the element. Then a preparatory program is used to edit the data from the analyzer and to rewrite them into a format compatible with the CDC-6600 computer. This computer is used for the spectral unfolding code. Finally, another program is used to extract data from the sequence of unfolded spectra to infer the spatial distributions of selected radionuclides.

6. **RESTRICTIONS AND LIMITATIONS**

   Analyses of spectra by this code are not influenced by the source geometry and no library of spectra is required. However, it is necessary to apply attenuation corrections to the results. These corrections are normally applied by other codes after the results of this code have been obtained.

   AMUSE can analyze up to 220 peaks in a single pass through one spectrum.

7. **TYPICAL RUNNING TIME**

   No study has been made by RSICC of typical running times for AMUSE.

8. **COMPUTER HARDWARE REQUIREMENTS**

   AMUSE is operable on the CDC 6600 computer.

9. **COMPUTER SOFTWARE REQUIREMENTS**
A Fortran 63 compiler is required.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in BCD card images; total records 1450.

12. DATE OF ABSTRACT
    November 1983.

    KEYWORDS:  GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
1. NAME AND TITLE
   **ANA**: Code System for Gamma-Ray Spectra Analyses.

   **AUXILIARY ROUTINES:**
   - **KATOK**: A Program for Resolving of Multiplets and Calculation of Peak Position, Net Area, FWHM and Their Uncertainties.
   - **RM**: A Utility for Displaying Text Files

2. CONTRIBUTORS
   Institute of Nuclear Research and Nuclear Energy, Sofia, Bulgaria, and International Atomic Energy Agency, Vienna, Austria.

3. CODING LANGUAGE AND COMPUTER
   - Borland C/C++ v3.1 and 8088 Assembler language; IBM PC's and compatibles (P00356/IBMPC/00).

4. NATURE OF PROBLEM SOLVED

5. METHOD OF SOLUTION
   - Energy calibration - line or parabolic approximation.
   - FWHM calibration - parabolic approximation; automatic peak search (based on first derivative method); calculation of first derivative using orthonormal polynomial approximation of the raw or smoothed spectrum.
   - Manual peak search - gives the experienced user the ability to correct the results of automatic peak search; resolving of multiplets and calculation of peak parameters (Gaussian peak shape, polynomial background approximation, normalized Gauss, Newton approximation method (KATOK).
   - Calculation of results for NAA - calculation of concentration of elements of interest in the sample and its uncertainty and/or calculation of LLD; background and dead time correction of required.
   - Efficiency calibration - spline method and polynomial approximation based on orthonormal polynomials.
   - Isotope identification - isotope library, user defined separation of analytical and additional isotope lines, background correction, calculation of LLD and MDC.

6. RESTRICTIONS OR LIMITATIONS
   Spectra formats supported - ORTEC, CANBERRA s-100, ACCUSPEC, IAEA ASCII format 'GANAAS'.
   - Spectrum length - from 512 to 8192 channels.
   - Energy calibration - from 2 to 20 peaks.
Efficiency calibration - from 3 to 20 peaks.
Maximum length of a single ROI - 500 channels. Maximum number of peaks in a ROI - 20,
maximum degree of background polynomial 4.
Number of ROIs in a spectrum is unlimited.
Efficiency calibration - from 2 to 20 peaks.

7. **TYPICAL RUNNING TIME**
   The time for calculation of peak parameters depends on complexity of the spectrum and specific
   PC hardware. On a 386 based machine with a math coprocessor a spectrum containing 140 peaks has
   been reduced to 25 seconds.

8. **COMPUTER HARDWARE REQUIREMENTS**
   ANA runs on an IBM PC or compatible with a 286 or greater processor. A math coprocessor is
   recommended but not required. At least 1.5 MB of disk space is required. An EGA or VGA graphics
   adapter is required and a color monitor is recommended.

9. **COMPUTER SOFTWARE REQUIREMENTS**
   Borland C/C++ v3.1 was used to compile the source code and create the executable included in
   the package.

10. **REFERENCE**

11. **CONTENTS OF CODE PACKAGE**
    The referenced document and 1 DS/HD 3.5" (1.44 MB) DOS diskette containing a self-
    extracting archive file are included. The archived file contains C source files, executables, sample
    input and output, and an information file.

12. **DATE OF ABSTRACT**
    July 1995.

    **KEYWORDS:** GAMMA-RAY SPECTRUM ANALYSIS; PLOTTING; MICROCOMPUTER
1. NAME AND TITLE
   **BOB-7 SERIES:** Theory and Use of Gamma-Ray Spectrum Analysis Codes for Ge(Li) Detectors.

2. CONTRIBUTOR
   Japan Atomic Energy Research Institute, Tokai Research Establishment, Ibaraki-ken, Japan.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; FACOM 230-60.

4. NATURE OF PROBLEM SOLVED
   BOB-7 SERIES analyzes the Ge(Li) gamma-ray spectrum and other types of spectra to determine the energies and intensities of the peaks detected. The spectrum is plotted in option.

5. METHOD OF SOLUTION
   The analysis is carried out by the photopeak method. The peak search is based on the first derivative method associated with various peak shape tests. The usual least squares method is adopted for resolving the complex of peaks. The line shape function as the basis of the fit is an asymmetric Gaussian with a tail; the asymmetry is realized with two half-Gaussian of different widths combined at the top. The shape of the base line under the peak can be selected out of the linear, exponential, and various stepwise functions.

6. RESTRICTIONS OR LIMITATIONS
   BOB-7 SERIES accepts a spectrum containing up to 200 peaks. The preferable spectrum size is 4100 or less, though larger data sizes are acceptable. The multiplicity of the complex of peaks should not exceed 18 in the case of “with tail” or 19 in the case of “without tail,” and the fitting range must be less than 200 channels.

   The pile-up effect appearing in the measurement at a high counting rate causes attenuation of the peak area. Correction for the effect is not considered in BOB-7 SERIES. The channel shift during the measurement is not corrected, either. BOB-7 SERIES does not require the accurate FWHM value as an input datum; a rough measure of the peak width is, however, still necessary.

7. TYPICAL RUNNING TIME
   The running time for BOB-7 SERIES depends upon the complexity of the spectrum rather than on the spectrum size. The analysis of a spectrum containing about 50 peaks with medium complexity (the maximum multiplicity among the complexes is about 5) requires approximately 10 seconds.

8. COMPUTER HARDWARE REQUIREMENTS
   BOB-7 SERIES is operable on the FACOM 230-60 computer. A 103 K word memory is required. A CALCOMP plotter, one or two magnetic tape units or a card puncher are optional.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.
10. REFERENCES

11. CONTENTS OF CODE PACKAGE
Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 17,119.

12. DATE OF ABSTRACT
March 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
1. NAME AND TITLE

**CERPI-CEREL:** Code Systems for Automatic Analysis of Gamma-Ray Spectra Obtained with Ge(Li) Detectors.

2. CONTRIBUTORS

Institute of Physics, University of Rome, Rome, Italy.
Comitato Nazionale per l'Energia Nucleare, Centro di Studi Nucleari della Casaccia, Roma, Italia.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; IBM 360/370.

4. NATURE OF PROBLEM SOLVED

CERPI and CEREL are automatic analyzers of gamma-ray spectra obtained with Ge(Li) detectors. CERPI analyzes experimental gamma-ray spectra in order to find the photopeak positions and areas. CEREL looks for those elements or nuclides which are potential emitters of the gamma-lines. It is possible to search by elements or nuclides, depending on the input parameter.

CERPI-CEREL contains features such as determination of peak energies and intensities, nuclide identification, and mass computation.

5. METHOD OF SOLUTION

CERPI detects the significant peaks in the spectrum by observing the behavior of the second derivative function after random variations in counts per channel have been minimized by the application of a smoothing filter function. Once the peaks have been identified, CERPI determines their mass centers, areas and corresponding errors with a least-squares fit. Each significant peak is fitted with a Gaussian function superimposed on a linear or quadratic background. The determination of the minimum of the $X^2$ function is accomplished by a variant of the gradient method.

CEREL does automatic isotope identification on the basis of gamma-ray energy comparison. It contains features such as determination of peak energies and intensities, nuclide identification, and mass computation. The energy calibration curve is determined starting from some known energy lines and by means of a fitting procedure with orthogonal polynomials using the F test for the automatic determination of the polynomial order. The single and double escape peaks are used for a more careful determination of the photopeak intensities and then removed from the observed spectrum. Pagden's isotope catalog is used for both nuclide identification and mass calculation.

6. RESTRICTIONS OR LIMITATIONS

The high precision and sensitivity of CERPI-CEREL make it very suitable to very complex spectrum analyses where many peaks overlap each other. This high sensitivity may imply the introduction of some spurious peaks. The higher the number of peaks identified, especially the number of spurious ones, the higher is the probability of introducing fictitious elements and the more complicated is the resolution of the mass matrix.

Particular care must also be taken in the choice of the input parameters because the fitting procedure is affected by this choice.
7. TYPICAL RUNNING TIME
   The running times of CERPI-CEREL depend strongly on the complexity of the spectrum and the number of channels in a typical peak. On an IBM 360/75 system, the analysis of a 4096-channel spectrum requires approximately 4 min of CPU processor time if about 250 peaks are printed on the final table.

8. COMPUTER HARDWARE REQUIREMENTS
   CERPI-CEREL is operable on the IBM 360/370 computers.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.

10. REFERENCES

11. CONTENTS OF CODE PACKAGE
    Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input, the isotope catalogue and the array listings written in EBCDIC card images, plus output from the sample problems written in list format; total records 12,333.

12. DATE OF ABSTRACT
    March 1984.

    KEYWORDS: ACTIVATION SPECTRA ANALYSIS; DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; GERMANIUM (Ge(Li)) DETECTOR; UNFOLDING
1. NAME AND TITLE
GAMAN: Qualitative and Quantitative Evaluation of Ge(Li) Gamma-Ray Spectra.

2. CONTRIBUTOR
Whiteshell Nuclear Research Establishment, Pinawa, Manitoba, Canada.

3. CODING LANGUAGE AND COMPUTER
Fortran IV and Assembler Language; PDP-10.

4. NATURE OF PROBLEM SOLVED
GAMAN does qualitative and quantitative analyses of gamma-ray spectra from Ge(Li) detectors.

5. METHOD OF SOLUTION
GAMAN "smooths" the spectral data by fitting 5 channel groups of data to a polynomial. The derivative is calculated at the midpoint of each group. A change of sign in the derivative indicates the beginning of a peak. The maximum and minimum values of the derivative are used to check on whether the peak height is statistically significant.

The significant peaks are fitted to a modified Gaussian function using a non-linear least squares procedure. This results in the calculation of the area and centroid of each peak and, by addition of calibration data, the gamma emission rates and energies are calculated and listed.

The listed energies are compared with gamma-ray energies in a library of isotopes and the isotopes present are identified.

The gamma-ray emission rate for each isotope is corrected for gamma-ray abundance and the disintegration rate is calculated.

6. RESTRICTIONS OR LIMITATIONS
None noted.

7. TYPICAL RUNNING TIME
GAMAN runs in < 120 seconds for 30 peaks.

8. COMPUTER HARDWARE REQUIREMENTS
GAMAN is operable on the PDP-10 computer. It requires 64 K of core memory.

9. COMPUTER SOFTWARE REQUIREMENTS
Fortran IV and Assembler Language compilers are required.

10. REFERENCES

11. CONTENTS OF CODE PACKAGE
Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in ASCII, plus output from the sample problem; total records 2550.

12. DATE OF ABSTRACT
February 1975.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
NEA CODE PACKAGE NESC9654/01

NESC9654 GAMANAL, RADIOACTIVE SPECIES MIX BY GAMMA SPECTRA ANAL 890116

1. NAME OR DESIGNATION OF PROGRAM - GAMANAL.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
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<th>Program-name</th>
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<th>Orig. Computer</th>
<th>Test Computer</th>
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<td>NESC9654/01</td>
<td>DEC VAX 11/750</td>
<td>DEC VAX 11/780</td>
<td>T</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

GAMANAL provides a complete qualitative and quantitative analysis of mixtures of radioactive species such as fission products by computer interpretation of high-resolution gamma-ray spectra. The program first determines and removes the background or Compton continuum under the peaks in a spectrum to locate the peak regions. This is done by examining the pulse-height spectrum data for background and peak regions and then fitting these data with the proper shape functions. When determining the photon emission rate, corrections are made for the effects of geometry, attenuation, and detector efficiency. Nonlinearities in the equipment are taken into account in setting up the energy scale. The total intensities and gamma-ray energies are listed and plotted and, if no further reduction of the spectral data is requested, the program repeats this process with the next spectrum. Otherwise, a library of decay scheme information is searched to make a tentative identification of each of the peaks. These proposed nuclides are examined for interferences between their photopeaks to determine which isotope is responsible for the peak in question. A matrix of the probable nuclides and the identified peaks is constructed and is then divided into sets of nuclides which interfere with each other. These independent sets are combined to form a working matrix. A least-squares solution of the corresponding set of simultaneous equations is made to determine the amounts of the various component nuclides present and their estimated errors.

4. METHOD OF SOLUTION

Peaks are located by a point-by-point examination of the first and second derivatives within the bounds of identified peak regions using statistically-weighted tests. Peak shapes are characterized by a shape analysis functions, which is the sum of a Gaussian and a tailing term. The data points in an overlapping peak multiplet are considered to be linear combinations of the contributions from each peak. A detailed analysis of each peak region is done by keeping some shape parameters fixed and obtaining the best least-squares value for all free parameters using the Newton-Raphson (Gauss) iterative technique. A Taylor expansion about trial values is used to linearize the equations. A matrix of linear equations that describe the spectral intensities is formed to correct for unresolved peak interferences. A Gaussian function is used to determine how well the component nuclide's gamma-ray energy agrees with the energy of the peak in question.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM
6. TYPICAL RUNNING TIME

NESC9654/01: NEA-DB ran the test case on a VAX-11/780 computer with the VERSAPLOT o/p plotter in 71 seconds of CPU time.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

LIBETP, an auxiliary program which is used to generate a GAMANAL decay-scheme library, is included. Graphic output is provided by DIGLIB and DIGRAPH, which are included. DIGLIB is a collection of FORTRAN-callable subroutines for two-dimensional plots. DIGRAPH acts as a shell for the GKS graphics routines.

9. STATUS

NESC9654/01: Known to NEADB
- Offered to NEADB
- Requested by NEADB
- Arrived at NEADB
- in preparation
- Tested at NEADB

10. REFERENCES

NESC9654/01:
- NEA Data Bank:
  Note Concerning Documentation of GAMANAL.
  NEADB Note (February 1988)
- C. Yuelys-Miksis:
  GAMANAL Tape Directory
  NESC Note 86-35 (April 15, 1986)
- R. Gunnink and J.B. Niday:
  Computerized Quantitative Analysis by Gamma-Ray Spectrometry.
  Volume I. Description of the GAMANAL Program.
  UCRL-51061, Vol. I (March 1, 1972)

  J.B. Niday and R. Gunnink:
  Computerized Quantitative Analysis by Gamma-Ray Spectrometry.
  Volume III. A User's Guide to GAMANAL.
  UCRL-51061, Vol. III (July 8, 1971)
  R. Gunnink and J.B. Niday:
  Computerized Quantitative Analysis by Gamma-Ray Spectrometry.
  Volume IV. Auxiliary Programs for GAMANAL.
  UCRL-51061, Vol. IV (June 1, 1972)
11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

NESC9654/01 : FORTRAN-77

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

VMS 4.2 (DEC VAX11/750), VMS 4.4 (DEC VAX11/780).

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

R. Gunnink
Lawrence Livermore National Laboratory
Livermore, California, U.S.A.

16. MATERIAL AVAILABLE

NESC9654/01 :
GAMANAL Source Code
DIGLIB Source Code
DIGRAPH Source Code
HELP File
Command Procedures
Sample Problem Input Data
Report: Machine Readable Documentation
GAMANAL Sample Output
NESC Note 86-35 (April 15, 1986)
NEADB Note (February 1988)
Report: UCRL-51061, Vol. 3 (July 8, 1971)
Report: UCRL-51061, Vol. 4 (June 1, 1972)

INFORMATION FILE
COMMAND FILE TO RESTORE ORIGINAL FILENAMES 330 records
HELP FILE 230 records
LIBRARY PROGRAM FORTRAN SOURCE 248 records
LIBRARY PROGRAM INPUT DATA 533 records
PERIODIC TABLE SYMBOLS 563 records
LIBRARY PROGRAM PRINTED OUTPUT LISTING 5 records
COMMAND FILE TO CREATE OBJECT LIBRARY 1586 records
COMMON STATEMENTS FORTRAN SOURCE 64 records
BGGPM.FOR FORTRAN SOURCE 229 records
BKGREG.FOR FORTRAN SOURCE 32 records
CALCMU.FOR FORTRAN SOURCE 509 records
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LOOKUP2.FOR FORTRAN SOURCE 488 records

17. CATEGORY = 0,

KEYWORDS Gauss function
Li-drifted Ge detectors
emission spectra
gamma spectra
isotopes
spectra unfolding
1. NAME AND TITLE

2. CONTRIBUTOR
   Atomic Energy Board, Pelindaba, Pretoria, Republic of South Africa, through the NEA Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran; IBM 360/370.

4. NATURE OF PROBLEM SOLVED
   GAMX1 evaluates accurate peak areas of gamma-ray and X-ray spectra generated by Ge(Li) and Si(Li) spectrometers. It renders accurate estimates of peak heights, position of centroids, and the backgrounds in the vicinity of the photopeaks being analyzed. However, it is intended to analyze spectra containing isolated peaks of known energy only; no facilities for peak location, energy calibration, or the analysis of doublets are included.

5. METHOD OF SOLUTION
   Photopeaks are analytically represented by a function composed of two Gaussians and an arc tangent superimposed upon a cubic polynomial background, thus ensuring the flexibility required for an authentic reproduction of X-ray and gamma-ray line shapes. This analytic peak function is applied to experimental spectra by virtue of the iterative Newton-Raphson non-linear least-squares fitting technique and the resulting set of equations is solved by pivotal condensation with back substitution. The empirical energy dependence of certain peak parameters is derived to enable the characteristics of the detection and measuring system to be quantified in terms of the energy dependence of the detector response before general spectra are analyzed. The quality of the fit to the photopeaks allows the uncertainty in each parameter and in the peak area to be computed. The error computed for the area of each individual peak is typically of the order of twice the uncertainty to be expected purely from statistics.

6. RESTRICTIONS OR LIMITATIONS
   Twelve previously analyzed GAMX1 peaks are employed in the present study, the energy of each photopeak (MeV) is 10F7.3, the parametric data pertaining to each photopeak is a set format, and the number of constants in each empirical equation is 411. The coefficients of the empirical parametric energy equations is a set format, the energy dependence of each parametric function in the sequence is 411, the number of peaks to be analyzed is 13, and a maximum of 200 data points exist for each spectrum.

7. TYPICAL RUNNING TIME
   No study has been made by RSICC of typical running times for GAMX1.

8. COMPUTER HARDWARE REQUIREMENTS
   GAMX1 is operable on the IBM 360/370 computers.
9. COMPUTER SOFTWARE REQUIREMENTS
A Fortran compiler is required.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in EBCDIC card images, plus output from the sample problem; total records 2079.

12. DATE OF ABSTRACT
November 1984.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; DETECTOR RESPONSE
1. NAME OR DESIGNATION OF PROGRAM. **GASPAN-ZKD**.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

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3. NATURE OF PHYSICAL PROBLEM SOLVED.

Analysis of gamma ray spectra obtained by a Ge(Li) detector and a multichannel pulse-height analyser to determine energy and intensity of gamma-lines.

4. METHOD OF SOLUTION.

After smoothing the spectral data (approximation to a power function by least squares method) domains with significant negative second differences are determined which mark the position of the peaks. A Gaussian function plus a quadratic function is fitted to each peak. The program allows identifying unresolved multiple peaks. It is possible to fit simultaneously up to 5 peaks.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.

Limited to spectra with 4096 channels and 100 peaks.

6. TYPICAL RUNNING TIME.

The running time depends on the number of channels and peaks and the demanded precision. The calculation for a spectrum with 1700 channels and 42 peaks requires 250 seconds of CPU-time. NEA-DB executed the test case on IBM 370/168 in 5 CPU seconds.

7. UNUSUAL FEATURES OF THE PROGRAM.

The programme uses an overly structure.

8. RELATED AND AUXILIARY PROGRAMS.

Random transfer system 'REX'.

9. STATUS

IAEA0877/01 : Arrived at NEADB
10. REFERENCES.

- B. Lindemann and M. Geisler: "GASPAN - A program for automatic evaluation of gamma spectra with the help of photo peak analysis," (in German) (December 1972)

11. MACHINE REQUIREMENTS.

400K bytes of main storage on IBM 370/168.

12. PROGRAMMING LANGUAGE USED

IAEA0877/01 : FORTRAN-IV

13. OPERATING SYSTEM OR MONITOR UNDER WHICH PROGRAM IS EXECUTED.

OS370/081 using the FORTRAN-H-EXTENDED compiler.

14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.

Input of the spectral data by perforated tape.

15. NAME AND ESTABLISHMENT OF AUTHOR.

B.Lindemann, M.Geisler
Zentralinstitut fuer Isotopen und Strahlenforschung
DDR 705 Leipzig
Permoserstrasse 15.

16. MATERIAL AVAILABLE

source program  mag tape
test-case data  mag tape
test-case output mag tape
GASPAN-ZKD INFORMATION FILE   41 records
GASPAN-ZKD SOURCE (FORTRAN-4)  45 records
17. CATEGORY = 0,

KEYWORDS Gauss function
Li-drifted Ge detectors
gamma detectors
gamma spectra
least square fit
multi-channel analysers
radiation detectors
1. NAME AND TITLE
   GAUSS: A Code system for Analysis of Gamma-Ray Spectra from Ge(Li) Spectrometers.

   GAUSS V (PSR-45A) was the original GAUSS package in the RSICC collection and was written for the IBM 360/75 computer. This original package was extended to include GAUSS VII (PSR-45B) which runs on the CDC computer. The two have now been combined into this one package and called GAUSS.

2. CONTRIBUTORS
   Aerojet Nuclear Company, Idaho Falls, Idaho (A).
   EG&G Idaho, Inc., Idaho Falls, Idaho (B).

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; IBM 360/370 (A) AND CDC (B).

4. NATURE OF PROBLEM SOLVED
   GAUSS determines gamma-ray energies and intensities from spectra obtained with a Ge(Li) detector and a multichannel pulse-height analysis system.

5. METHOD OF SOLUTION
   The preliminary portions of the program can determine the energy and width calibration equations, locate individual peaks and define “peak regions” that are significantly above the local spectral background. The user may edit these lists of peaks and regions. Each peak region is fitted with one or more components in which the peaks are represented by a Gaussian function or a Gaussian with one or two additive exponential tails on the low-energy side and one on the high-energy side. A step-like background function can be used with each component. The program will automatically recycle to add one or more components to a region if needed to improve the fit. The gamma-ray energies and intensities are computed from the resulting Gaussian positions and peak areas. To allow the user to determine the best results, the results from the analyses for each region with different numbers of components can be printed and line-printer plots of the fits to the data can be made.

6. RESTRICTIONS OR LIMITATIONS
   GAUSS will handle spectra of up to 4096 channels with up to 300 peaks and 50 energy calibration lines.

   The quality of the results depends primarily on the ability of the program to define a good spectral region for each analysis and the ability to recycle to determine the proper number of components.

7. TYPICAL RUNNING TIME
   Typical spectra can be analyzed at a rate of approximately 5 per minute.

8. COMPUTER HARDWARE REQUIREMENTS
   GAUSS is operable on the IBM 360/370 computer (A) or the CDC computer (B). A printer and
punch are required.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran compiler is required.

10. REFERENCES

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and a reel of magnetic tape which contains the source codes and sample problem input written in EBCDIC card images, plus output from the sample problem written in list format; total records 4960 (A) or 13,591 (B).

12. DATE OF ABSTRACT
    October 1983.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
NEA CODE PACKAGE NESC0622/01

NESC0622 GAUSS-6, EXPERIMENTAL GAMMA_SPECTRA ANALYSIS, ISOTOPE_IDENTIFICATION, DECAY_RATES 801117

1. NAME OR DESIGNATION OF PROGRAM - **GAUSS6**

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

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3. DESCRIPTION OF PROBLEM OR FUNCTION

GAUSS6 is used for the production analysis of gamma-ray spectra obtained with a Ge(Li) detector and a multichannel pulse-height analyzer system. In addition to determining gamma-ray energies and intensities, it provides isotopic identification, decay corrections and correlation of data from different peaks and different spectra to obtain isotopic decay rates.

4. METHOD OF SOLUTION

- GAUSS6 carries out the following steps -
  (a) Sorts master nuclide library to obtain a subset including only the nuclides of interest.
  (b) Automatically locates peaks by means of an auto-correlation routine.
  (c) Fits each peak with a Gaussian function plus a linear function representing the spectral background. Only the three Gaussian parameters (height, width, and position) are allowed to vary. The fit extends down to 1.5 times the width of the Gaussian (FWHM). Fits that fail to converge are repeated with a fixed width.
  (d) Determines peak width and energy calibration functions from a Th228 spectrum. These functions as well as the energy calibration from any spectrum can be transferred to subsequent spectra.
  (e) Attempts isotopic assignments for all peaks. Decay corrections are made.
  (f) For spectra from the same sample, edits and averages the results to obtain the isotopic decay rates.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

GAUSS6 will handle any number of spectra of up to 4096 channels with up to 300 peaks and 20 energy calibration lines. The subset of the isotopic library is limited to 1000 gamma rays.

6. TYPICAL RUNNING TIME

Typical spectra can be analyzed at a rate of about 5 per minute.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS
The program package includes the following auxiliary programs:

(a) LCTAPE for putting nonlinearity correction and efficiency tables on disk.
(b) UPDATE for updating the master nuclide library.
(c) RASLIB for producing a subset of the master nuclide library (normally run as part of the analysis run).
(d) MERGE for combining the output tapes from several GAUSS6 analyses.
(e) CORLAT for carrying out the comparison and averaging of the several measurements for each sample.
(f) LIBRER for generating a nuclide library data set from cards.
(g) SECLIB for generating a secondary library subset for CORLAT.

GAUSS6 is based on GAUSS5 (NESC Abstract 605), but is written to analyze large groups of spectra efficiently and includes calculations beyond the gamma-ray energies and intensities and can compare results from different gamma-rays and different spectra to verify nuclide assignments for individual peaks.

9. STATUS

NESC0622/01: Arrived at NEADB
   : in preparation
   : Tested at NEADB

10. REFERENCES

    GAUSS6, ACC No. 622, Argonne Code Center Programming Note 74-29, March 29, 1974.

11. MACHINE REQUIREMENTS

    GAUSS6 requires storage devices for the spectral library, nuclide library subset, and the correlation data in addition to three scratch devices and the card reader and printer. CORLAT requires storage devices for the secondary library subset and the correlation data plus four scratch devices and the card reader and printer.

12. PROGRAMMING LANGUAGE USED

    NESC0622/01: FORTRAN-IV

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

    OS/360 MVT.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

    The CORLAT program requires the IBM360 SORT package.
15. NAME AND ESTABLISHMENT OF AUTHORS

R. G. Helmer, J. E. Cline, and M. H. Putnam
EG&G Idaho, Inc.
P. O. Box 1625
Idaho Falls, Idaho 83401

16. MATERIAL AVAILABLE

NESC0622/01:

Report:
INFORMATION 1 records
LIBRER PROGRAM SOURCE (PL/1) 182 records
SAMPLE PROBLEM DATA 10 records
SAMPLE PROBLEM PRINTED OUTPUT 27 records
EXECUTION DD CARDS 4 records
LCTAPE PROGRAM SOURCE (F4) 170 records
SAMPLE PROBLEM DATA 60 records
SAMPLE PROBLEM PRINTED OUTPUT 140 records
EXECUTION DD CARDS 2 records
RASLIB PROGRAM SOURCE (PL/1) 461 records
SAMPLE PROBLEM DATA 5 records
SAMPLE PROBLEM PRINTED OUTPUT 28 records
EXECUTION DD CARDS 4 records
GAUSS-6 SOURCE MODULE (BAL) 2811 records
GAUSS-6 SOURCE MODULE (F4) 3825 records
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SAMPLE PROBLEM PRINTED OUTPUT 1043 records
EXECUTION DD CARDS 14 records
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SAMPLE PROBLEM DATA 1 record
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UPDATE PROGRAM SOURCE (PL/1) 518 records
SAMPLE JCL 9 records

17. CATEGORY = O,

KEYWORDS Li-drifted Ge detectors
gamma spectra
isotopes
1. NAME AND TITLE
   GRETEL: Analyzer and Processor of Ge(Li) Gamma-Ray Spectrometric Data.

2. CONTRIBUTOR
   Joint Nuclear Research Centre, Ispra Establishment (EURATOM), Ispra, Italy.
   OECD Nuclear Energy Agency Computer Program Library, Ispra, Italy.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV and Assembler language; IBM 370.

4. NATURE OF PROBLEM SOLVED
   GRETEL performs the quantitative analysis of gamma-ray spectra obtained by Ge(Li) detectors using special "oriented libraries" which are prepared for each particular problem.

5. METHOD OF SOLUTION
   The computer routines which detect and evaluate peak areas perform the following operations: 1) local smoothing of the spectrum, 2) first derivative of the smoothed spectrum, 3) peak location according to the change of sign of the first derivative, 4) computation of the net area of each peak found. GRETEL can also detect and compute double peaks from a study of the behavior of the first derivative.
   An energy calibration source is counted by GRETEL as the first spectrum of the series; then the unknown neutron activated samples are successively counted. The analysis is carried out by the single comparator method. Irradiation and decay times, weight of samples and neutron flux are manually assigned by the operator. Peaks in the gamma spectrum are searched, identified and measured by following the instructions of special "oriented" libraries which are prepared for each particular problem.

6. RESTRICTIONS OR LIMITATIONS
   The maximum number of calibration peaks is 10. The maximum number of elements of the "oriented library" is 50. The maximum number of channels of the spectrometer which can be used is 4096. No limitation exists on the number of spectra to be treated. It is imperative that the calibration spectrum is always the first of the set.
   CALCOMP plotting must be requested separately after the complete running of the program.

7. TYPICAL RUNNING TIME
   For a typical analysis of 30 spectra of 2048 channels (calibration spectrum plus 29 unknown), with an "oriented library" of 30 elements, the running time is about 30 seconds (object program).

8. COMPUTER HARDWARE REQUIREMENTS
   GRETEL is operable on the IBM 370 computers. The plotting routines are for a CALCOMP 900 off-line plotter.

9. COMPUTER SOFTWARE REQUIREMENTS
   Fortran IV-G and Assembler language compilers are required.
10. REFERENCE
   G. Guzzi and J. Cuypers, “GRETEL, A Computer Program for Gamma Ray Spectrometry with

11. CONTENTS OF CODE PACKAGE
   Included are the referenced documents and a reel of magnetic tape which contains the source
   code and sample problem input written in EBCDIC card images, the plotting subroutines written in
   Fortran IV and Assembler Language, plus the output from the sample problem written in list format;
   total records 11,034.

12. DATE OF ABSTRACT
   March 1984.

   KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
RSICC CODE PACKAGE PSR-321
NEA CODE PACKAGE PSR-0321

1. NAME AND TITLE
   GRPANL: Code System for Analyzing Ge and Alpha-Particle Detector Spectra.

2. CONTRIBUTORS
   Lawrence Livermore National Laboratory, Livermore, California through the Energy Science &
   Technology Software Center, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER/OPERATING SYSTEM
   Fortran 77; VMS 4.7

4. NATURE OF PROBLEM SOLVED
   GRPANL (GRouP ANaLysis) is a suite of programs which analyzes and interprets regions of
   germanium and alpha-particle detector pulse-height spectra. GRPANL is the main peak-fitting
   program; the other programs included are used in conjunction with GRPANL. GRPANL is
   particularly useful for accurately deconvoluting and interpreting complex clusters of peaks in a
   spectrum. GRPANL fits peaks in specified regions of a gamma-ray, x-ray, or alpha-particle
   spectrum, calculates their energies and intensities, and optionally calculates the photon emission
   rates for the sample from which they were emitted. It can also identify and measure isotopes in a
   sample. GRPANL output can be immediately analyzed for quantitative isotopic assays or stored in
   an intermediate data file. The other programs are EDIGRP, LIBRY, and GEVAL. EDISRP (EDIt
   GRouP) creates and edits an analysis control file that contains input parameters and analysis options
   for spectral regions analyzed by GRPANL; users can repeat or modify an analysis without retyping
   input. LIBRY (LIBRarY) assembles and cross references selected nuclear decay scheme data and
   stores it in decay scheme data files for use by GRPANL and GEVAL. GEVAL (Gamma ray
   EVALuation) uses these data files along with GRPANL intermediate results to identify isotopes,
   calculate their abundance in a sample, and print the corresponding disintegration rates and
   abundances at counting and zero times.

5. METHOD OF SOLUTION
   The peaks in any x-ray or gamma-ray spectrum are always superimposed on a background
   distribution resulting from the Compton scattering process. GRPANL first removes the background
   continuum before starting the fitting process thus reducing the number of fitting parameters.
   GRPANL then estimates the initial peak heights and positions. The Gauss-Seidel, or Newton-
   Raphson, iterative least-squares technique is applied to fit the data because the equations describing
   the peak-shape are nonlinear in form. Convergence is determined by comparing the magnitude of the
   last change in each variable with a specified convergence criterion.
   Once convergence is attained, fuel calculations are made for peak energies, intensities, and their
   respective uncertainties. The intensity uncertainties are based on counting statistics and on the
   goodness-of-fit.

6. RESTRICTIONS OR LIMITATIONS
   Maxima of 1024 channels per peak, 40 degrees of freedom, and 40 peaks. GEVAL can evaluate
   a maximum of 200 peaks. The auxiliary programs CALDET, XDIST, LLFIT, and PKSHAP
   described in the reference reports are not included in the package. CALDET is used as an aid in
calibrating a new detector. LLFIT fits an nth order polynomial to the data and reports the coefficients of the fit. These coefficients may then be stored in the detector coefficients file for subsequent analysis using this newly calibrated detector.

7. TYPICAL RUNNING TIME
The programs are interactive.

8. COMPUTER HARDWARE REQUIREMENTS
The codes run on the VAX family of computers.

9. COMPUTER SOFTWARE REQUIREMENTS
GRPANL uses the LLNL DIGRAPH and DIGLIB codes to produce graphical output. These programs are supplied in object form only. The VMS Fortran compiler was used on the VMS operating system.

10. REFERENCES
a: included in document:
GRPANL Sample Output (September 1988).

b: background information:

11. CONTENTS OF CODE PACKAGE
Included in the package are the referenced documents and 1 DS/HD disk which includes the source files, test case input data and output.

12. DATE OF ABSTRACT

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE; PARAMETRIC MODELS; PLOTTING; UNFOLDING
1. NAME AND TITLE

**HYPERMET**: Gamma-Ray Spectra Analyzer Germanium Detector

2. CONTRIBUTOR

Naval Research Laboratory, Washington, D. C.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; CDC 3800 (A), T. I. ASC-7 IBM COMPATIBLE (B), FACOM M190 (C).

4. NATURE OF PROBLEM SOLVED

HYPERMET performs an automatic analysis of a multichannel gamma-ray pulse-height spectrum taken with a germanium detector. It has a number of options including an energy calibration, correction for radioactive decay, and a CALCOMP plot of each fit.

5. METHOD OF SOLUTION

A peak search is done by using a zero-area sliding transform on the data. A peak is indicated by a rise above a preset threshold. A fitting subregion is then defined about the peak and initial values are determined for the parameters of a semi-empirical peak-shape function plus background. Within this subregion, initial estimates are made for the parameters such as background level.

An iterative non-linear least-squares fit is done for the optimum values of the parameters. If programmed criteria for a good fit are not satisfied, the residuals (data minus fit) are searched for indication of an additional peak in the data. If found, the fit is repeated with the additional peak included.

6. RESTRICTIONS OR LIMITATIONS

HYPERMET is dimensioned for up to 8192 channel spectra with up to 100 peaks per spectrum.

7. TYPICAL RUNNING TIME

Running time varies linearly with peak width and quadratically with the number of multiplet peaks which must be fit simultaneously. Spectra with poor statistics are fit more rapidly than those with good statistics for which the statistical criteria for a good fit are more stringent.

For a typical spectrum with peak widths from 3 to 5 channels FWHM, moderate statistics, and mostly well separated peaks, running time on the CDC 3800 computer is on the order of one minute for every ten peaks in the spectrum.

8. COMPUTER HARDWARE REQUIREMENTS

HYPERMET is operable on the CDC 3800 (A), T. I. ASC-7 (B), or the FACOM M190 computers. Except for a few system input-output routines, it will fit into one 32 K word bank on a CDC 3800 computer.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran IV compiler is required.

10. REFERENCES
11. CONTENTS OF CODE PACKAGE

Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in BCD/EBCDIC/ASC card images, plus output from the sample problem; total records 4490 (A), 7145 (B), and 4001 (C).

12. DATE OF ABSTRACT

March 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; GERMANIUM (Ge(Li)) DETECTOR; PLOTTING; UNFOLDING
1. NAME OR DESIGNATION OF PROGRAM - JADSPE.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>JADSPE</td>
<td>IAEA0940/01</td>
<td>ICL 4/72</td>
<td>ICL 4/72</td>
<td>A</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

JADSPE is a package of eight programs to process multichannel gamma-ray spectra. The programs can be used to:
- locate automatically spectral peaks and calculate their positions, areas, and full widths at half maximum (FWHM);
- plot the spectra on a CALCOMP plotter, TEKTRONIX terminal or a line printer;
- add or subtract several spectra with the possibility of adjusting either their start and end channels or the maxima of the chosen corresponding peaks.

The JADSPE package comprises the following programs:

SPECTF: automatic location of peaks and calculation of their positions, areas and FWHMs. The standard deviations of peak parameters are also determined, and each evaluated region is plotted on the line printer.

SPECT1: The areas and FWHMs are calculated for peaks whose positions are known beforehand. The standard deviations of calculated parameters are also determined, and each evaluated region is plotted on the line printer.

PLOCHA: The peak net area is calculated by summing the channel contents in specified regions and by subtracting a linear background.

GRAPH: Spectrum plotting on the line printer.

PLTNEW: Spectrum plotting on CALCOMP plotter or on TEKTRONIX terminal.

SUMDIF: The channel contents of several gamma-ray spectra are added or subtracted.

SSPFP: The channel contents of several gamma-ray spectra are added with adjustment of the maxima of specified peaks.

SOUCET: The channel contents of several gamma-ray spectra are added with the adjustment of start and
end channels of the spectra.

4. METHOD OF SOLUTION

Non-linear least-square fit.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

The full energy peaks are approximated by a symmetrical Gaussian function and the underlying background is approximated by a first-order polynomial. A fixed spectrum length of 4096 channels is assumed.

Maxima of:
- number of peaks in one multiplet: 9
- number of peaks identified by the automatic search procedure: 300
- number of channels in one evaluated interval: 500
- dimensions of CALCOMP plots: 54 cm x 36 cm
- number of spectra, which may be added by SSPFP: 5
- number of peaks for spectra adjustment in SSPFP: 20
- number of spectra added by SOUCET: 10.

6. TYPICAL RUNNING TIME

SPECTF, SPECT1: running time depends on the spectrum complexity and the total number of peaks evaluated. The determination of peak positions, areas, and FWHM's requires from 10 to 60 ETU per spectrum (1 ETU = 3.6 seconds).

GRAPH: plotting on line printer requires about 25 ETU per spectrum.

PLTNEW: plotting on CALCOMP requires about 2 ETU per spectrum.

SUMDIF, SSPFP, SOUCET: running time depends on the number of spectra involved. To sum two spectra requires about 4 ETU.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

IAEA0940/01: Requested by NEADB
            : Arrived at NEADB

10. REFERENCES

- J. Pitha, R.N. Jones: Internal Report Division of Pure Chemistry, National Research Council, Ottawa Canada
- "Multijob Programming" TP4572, ICL
11. MACHINE REQUIREMENTS

Program execution requires from 41 to 106 bytes of mainm storage. CALCOMP plotter or TEKTRONIX 4010 terminal are required for spectrum plotting.

12. PROGRAMMING LANGUAGE USED

IAEA0940/01 : FORTRAN-IV

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

MULTIJOB (ICL/4-72)

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

J. RIKOVSKA and E. STEJSKALOVA
Technical University of Prague
Faculty of Nuclear Science and Physical Engineering
Department of Mathematics
Brehova 7
115 19 PRAGUE 1 - Stare Mesto
CZECHOSLOVAKIA

16. MATERIAL AVAILABLE

SPECTF Source program
SPECTF JCL
SPECTF Sample Problem Input Data
SPECTF Source program
SPECTF JCL
SPECTF Sample Problem Input Data
PLOCHA Source program
PLOCHA Macro (USERCODE)
PLOCHA JCL
PLOCHA Sample Problem Input Data
PLOCHA Sample Problem Input Data S0019
PLOCHA Sample Problem Printed Output
GRAPH Source program
GRAPH JCL
GRAPH Sample Problem Input Data
PLTNEW Source program
PLTNEW JCL
PLTNEW Sample Problem Input Data
SUMDIF Source program
SUMDIF JCL
SUMDIF Sample Problem Input Data
SUMDIF Sample Problem Printed Output
SSPFP Source program
SSPFP JCL
SSPFP Sample Problem Input Data
SSPFP Sample Problem Printed Output
SOUCEt Source program
SOUCEt JCL
SOUCEt Sample Problem Input Data
SOUCEt Sample Problem Printed Output
SPECTF Sample Problem Printed Output
SPECT1 Sample Problem Printed Output
GRAPH Sample Problem Printed Output
Report: JADSPE Report (December 1987)

17. CATEGORY = N, O,

KEYWORDS data processing
gamma detectors
gamma spectra
least square fit
multi-channel analysers
spectra unfolding
NEA CODE PACKAGE NESC9580

NESC9580 RICKI, INTERACTIVE GAMMA SPECTRA UNFOLDING WITH ISOTOPE IDENTIFICATION 900918

1. NAME OR DESIGNATION OF PROGRAM - RICKI.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>RICKI</td>
<td>NESC9580/01</td>
<td>IBM PC</td>
<td>IBM PC</td>
<td>T</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

RICKI is an interactive program for analysis of gamma spectra containing one or more peaks with possible multiplets. Algorithms are incorporated for peak fitting, analysis, and nuclide identification. Comprehensive output keeps the user informed of the analysis as it proceeds and presents the results. User-selectable options for plotting and neutron activation analysis are available to control this analysis. RICKI was developed to analyze spectra from examinations of severe fuel damage specimens. Two features included to streamline the analysis of Three Mile Island (TMI) core bore data are the edit of averaged activities and the output file created for generating a spreadsheet. Activity editing allows the user to select which gamma lines are used for a specific nuclide in average activity calculations. Contributions from peak areas which result from overlapping lines of two or more nuclides may be removed. For each averaged activity an edited activity file record is written containing the nuclide name, averaged activity, activity standard deviation, scan start position, and scan end position.

4. METHOD OF SOLUTION

The peak search algorithm utilizes an optimized second derivative filter for efficient and reliable determination of peak location. A linear Gaussian fitting technique, which is a modified version of Mukoyama's linear least squares fitting method in which the centroid, sigma, and peak height are free parameters, is used to calculate peak areas. An estimated background is computed for each peak using Gunnink's method. Nuclide activities are computed by matching centroids with nuclide library entries and averaging the activity calculated for each matching peak.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Maxima of - 500 gamma library entries 80 peaks/spectrum

6. TYPICAL RUNNING TIME

Running time varies from 20 seconds to 5 minutes.
7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

RICKI was developed from CINA, a simpler fitting and peak integration program. The CINA gamma line library and menu sections are retained in RICKI. Auxiliary programs GAMLIB, EFFCAL, and SPECMOD provide gamma library maintenance, detector efficiency table generation, and spectrum error correction, respectively. Auxiliary program CORESORT converts TMI core bore scan data to the format of a listing of activity versus scan position for each nuclide and produces a spreadsheet input file (nuclide activity listed by scan position) readable by LOTUS 1-2-3. RICKI is not intended to replace large-scale gamma analysis codes such as GAUSS8, GAMANAL (NESC 9654), or SAMPO, but provides rapid, accurate analysis for cases where detailed peak shapes and other parameters may not be known.

9. STATUS

NESC9580/01: Offered to NEADB
- Requested by NEADB
- Arrived "as is"
- in preparation
- Tested at NEADB

10. REFERENCES

NESC9580/01:
- M. Birgersson: "RICKI Flexible Disk Cartridge Description and Implementation Information," NESC Note 88-27 (December 31, 1987)

11. MACHINE REQUIREMENTS

An IBM PC, preferably equipped with math coprocessor and an enhanced graphics adapter, a minimum of two floppy disk drives, and an EPSON FX-286 or compatible printer for graphics printing. A hard disk is desirable to obtain reasonable nuclide sorting time.

NESC9580/01: Main storage requirements on an IBM PC/AT are as follows: RICKI and RICKI2: 175K; GAMLIB: 75K; EFFCAL: 95K; SPECMOD: 90K; CORESORT: 50K.

12. PROGRAMMING LANGUAGE USED

NESC9580/01: BASIC
13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

DOS 3.1.
NESC9580/01: The program ran under MSDOS version 3.30. The compiler Microsoft QuickBASIC version 4.00 and linker Microsoft Linker 3.63.08 were used.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

Because some DOS systems do not allow more than three open files, two RICKI source files are provided. RICKI2 edits the averaged activities and procedures output file (the fourth open file) for use by the CORESORT spreadsheet generation program. RICKI, which does not perform this editing, opens only three files.

15. NAME AND ESTABLISHMENT OF AUTHORS

A.E. Proctor
EG&G Idaho, Inc.

16. MATERIAL AVAILABLE

NESC9580/01:
TMISPEC.PAR Menu file containing parameters
THORIUM.LIB Thorium library
TMIPEAKS.LIB TMI peak identification lib.
CALIB.LIB Calibration library
RICKI.BAS RICKI source
RICKI.MAP RICKI load map
.RICKI.EXE RICKI executable file
TABLE.EFF Efficiency table
GAMLIB.BAS GAMLIB BASIC source
CORE.EFF Core efficiency table
GAMLIB.LST GAMLIB compilation listing
GAMLIB.MAP GAMLIB load map
GAMLIB.EXE GAMLIB executable file
TEST.EFF Demonstration efficiency table
.EFFCAL.BAS EFFCAL BASIC source
.EFFCAL.LST EFFCAL compilation listing
.EFFCALL.MAP EFFCAL load map
.EFFCAL.EXE EFFCAL executable file
CALIB.EFF Calibration efficiency table
TEST.PAR Test parameter
RODS.EFF Efficiency table for rods
PETE.EFF Test efficiency table for rods
.SPECMOD.BAS SPECMOD BASIC source
SPECMOD.LST SPECMOD compilation listing
SPECMOD.MAP SPECMOD load map
SPECMOD.EXE SPECMOD executable file
RICKI2.BAS RICKI2 BASIC source
CORESORT.BAS CORESORT BASIC source
RICKI2.EXE RICKI2 executable file
CORESORT.EXE CORESORT executable file
GAMLIB.SC1 Gamma library spectrum file 1
GAMLIB.SC2 Gamma library spectrum file 2
86240001.GSR Spectral data file
86240003.GSR Spectral data file
Report: EG&G Idaho (October 1986)
NESC Note 88-27 (December 31, 1987)
Report: EGG-PHY-7545 (February 1987)
Report: EGG-PHY-7545 ADDENDUM
Information file
Spectral data file
Spectral data file
Calibration efficiency table
Calibration library
Core efficiency table
CORESORT BASIC source
CORESORT executable file
EFFCAL BASIC source
EFFCAL executable file
EFFCAL compilation listing
EFFCAL load map
GAMLIB BASIC source
GAMLIB executable file
GAMLIB compilation listing
GAMLIB load map
Gamma library spectrum calculation file 1
Gamma library spectrum calculation file 2
Test efficiency table for rods
RICKI BASIC source
RICKI executable file
RICKI load map
RICKI2 BASIC source
RICKI2 executable module
Rod efficiency table with Ce/Eu strip stand.
SPECMOD BASIC source
SPECMOD executable file
SPECMOD compiling listing
SPECMOD load map
Efficiency table
Demonstration efficiency table
Test parameter file
Thorium library
TMI peak identification library
File containing parameters for spect. anal.

133 records
848 records
848 records
21 records
0 records
11 records
401 records
0 records
884 records
0 records
1038 records
25 records
705 records
0 records
811 records
25 records
0 records
9 records
20 records
2297 records
0 records
2364 records
0 records
20 records
918 records
0 records
1075 records
25 records
1 records
7 records
19 records
0 records
0 records
19 records

52
DOS file-names

17. CATEGORY = 0,

KEYWORDS Gauss function
activation analysis
gamma spectra
spectra unfolding
1. NAME AND TITLE

SAMPO-LRC: Gamma-Ray Spectrum Analysis Code.

SAMPO, originally called SISYPHUS, was developed on the CDC 6600 computer at the Lawrence Berkeley Laboratory at the University of California in 1969 in support of the author's doctoral dissertation. The IDENT subroutine included in this version carries out radioisotope identifications and elemental mass determinations after simple or cyclic thermal-neutron activation analysis. A minicomputer version of the code, PSR-204/SAMPO-80, was developed at the Helsinki University of Technology, Nuclear Engineering Laboratory, Finland.

2. CONTRIBUTOR

University of London Reactor Centre, Berkshire, England.

3. CODING LANGUAGE AND COMPUTER

Fortran IV; CDC 6600.

4. NATURE OF PROBLEM SOLVED

SAMPO is a versatile gamma-ray spectrum analysis program used for the analysis of the complex spectra encountered in neutron-activation analysis. In particular, it is intended for photo-peak analysis of gamma-ray spectra obtained with semiconductor detectors. It includes routines for peak-finding, peak-fitting and peak intensity and energy determinations. It also makes complete statistical and calibration-error estimates. Different options are available to make the code applicable to accurate nuclear spectroscopic work as well as routine data reduction.

5. METHOD OF SOLUTION

SAMPO contains a mathematical formalism for the representation of photopeaks and the continua in their vicinity which is applicable to analysis of spectra measured under widely varying conditions. With this formalism, the line shape is defined for each peak in the spectrum. The region of data about a single peak is then fitted with the shape functions and a function representing the background continuum. The line-shape calculations and the fitting are performed by using a least-squares procedure with an iterative gradient minimization method with variable metric.

IDENT, a subroutine of SAMPO, carries out radioisotope identifications and elemental mass determinations after simple or cyclic thermal-neutron activation analysis by matching the peaks found with its nuclear data library.

6. RESTRICTIONS OR LIMITATIONS

IDENT is dimensioned to allow for a maximum of 15 peaks in any one interval and 50 unsuccessful identifications in each spectrum. These limits may be increased if necessary.

7. TYPICAL RUNNING TIME

No study has been made by RSICC of typical running times for SAMPO.

8. COMPUTER HARDWARE REQUIREMENTS

SAMPO was designed to run on the CDC 6600 computer.
9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.

10. REFERENCES
   a. Included in the documentation:

   b. Background information:

11. CONTENTS OF CODE PACKAGE
    Included are the referenced documents and a reel of magnetic tape which contains the source codes, sample problem input, and JCL for the CDC 6600 written in EBCDIC card images, plus output from the sample problem; total records 7929.

12. DATE OF ABSTRACT
    June 1982; revised October 1983; updated January 1984; revised April 1984; reviewed May 1984.

    KEYWORDS: ACTIVATION SPECTRA ANALYSIS; GAMMA-RAY SPECTRUM ANALYSIS; GERMANIUM (Ge(Li)) DETECTOR
RSICC CODE PACKAGE PSR-204
NEA CODE PACKAGE NEA-0691

1. NAME AND TITLE

SAMPO80: Gamma-Ray Spectrum Analysis Method for Minicomputers.

AUXILIARY ROUTINES

SAMPOSHAPE: Performs peak shape calibration.
SAMPOFIT: Performs peak search and fitting.
SAMPOID: Performs nuclide identification.

SAMPO, originally called Sisyphus, was developed on the CDC 6600 computer at the Lawrence Berkeley Laboratory of the University of California in 1969 in support of the author's doctoral dissertation. The analysis methods employed in this minicomputer version are simplified from those in the original code. Another version of this code, PSR-186/SAMPO-LRC, was modified at the London Reactor Centre and runs on the CDC 6600 computer.

2. CONTRIBUTORS

Helsinki University of Technology, Nuclear Engineering Laboratory, Espoo, Finland.
OECD Nuclear Energy Agency Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER

Fortran 5; Data General Nova 2.

4. NATURE OF PROBLEM SOLVED

SAMPO80 is a rapid and accurate analysis program for gamma-ray spectra measured with Ge(Li) or HPGe detectors. SAMPO80 consists of three separate parts, the shape calibration part SAMPOSHAPE, the peak search and fitting part SAMPOFIT, and the nuclide identification part SAMPOID.

5. METHOD OF SOLUTION

The shape calibration procedure uses a non-linear least squares algorithm with a variable metric method. Some other features include: peak location with a smoothed second difference method, peak area calculation with a linear least squares fit to predefined peak shapes, and nuclide identification with a linear least squares fit based on associated lines.

6. RESTRICTIONS OR LIMITATIONS

- Number of shape calibration points allowed: 20
- Number of energy calibration points allowed: 20
- Number of efficiency calibration points allowed: 20
- Maximum number of found peaks: 100
- Maximum number of fitted peaks: 100
- Maximum number of peaks in a multiplet: 5
- Maximum number of channels in a fitting interval: 50
- Maximum number of peaks for nuclide identification: 80
- Maximum number of identified nuclides: 30
- Maximum number of lines per nuclide: 30
7. **TYPICAL RUNNING TIME**
On a Data General Eclipse S/140 with microcoded floating point instruction set, 25 seconds are required per shape calibration of one peak, 2 seconds per peak for peak search and fitting, and 3 seconds per identified nuclide for identification.

8. **COMPUTER HARDWARE REQUIREMENTS**
SAMPO80 is operable on the Data General Nova 2 minicomputer with a 32 kiloword central memory and a supporting disk unit.

9. **COMPUTER SOFTWARE REQUIREMENTS**
This version of SAMPO80 is run under the Data General Real Time Disk Operating System (RDOS) and requires a Fortran 5 compiler.

10. **REFERENCES**

11. **CONTENTS OF CODE PACKAGE**
Included are the referenced documents and a reel of magnetic tape which contains the source codes, sample problem input, and console dialogue written in EBCDIC card images, plus output from the sample problem; total records 4615.

12. **DATE OF ABSTRACT**

**KEYWORDS:** ACTIVATION SPECTRA ANALYSIS; GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE
SKEWGAUS: Skewed-Gaussian Line Peak Fitting Code — Multichannel Analyzer (MCA) Spectra — Ge(Li) and Semiconductor Detectors.

Ames Laboratory, USDOE, Iowa State University, Ames, Iowa.

Fortran IV, PL/I; IBM 360/370.

SKEWGAUS fits a skewed-Gaussian line shape to peaks in multichannel analyzer (MCA) spectra obtained with Ge(Li) and Si(Li) semiconductor detectors.

SKEWGAUS reads an entire multichannel analyzer (MCA) spectrum and retains this spectrum in core while all fits are being performed on it. Any number of fits may be performed on a spectrum and any number of spectra may be included in a single execution of the program. Each fit may include a superposition of up to nine peaks in addition to a linear or (optionally) quadratic background. Parameters of different peaks may be constrained to vary proportionately during the fit. Different convergence criteria are applied to different peak parameters. Several options are available for handling the background, permitting it to be fit either concurrently with the peaks or separately. A modified statistical weighting of the MCA data points takes into account the differential non-linearity of the analyzer. SKEWGAUS was designed to supply its own initial estimates for nearly all parameters so that the amount of input data which must be supplied is minimal.

The maximum number of channels included in the channel-by-channel output listing is 210; the maximum number of variable parameters in a fit is 40. It is possible to change these numbers following instructions in the documentation.

The maximum number of peaks in a fit is 9. This number cannot be changed easily.

On an IBM 360/65 system, a sample problem involving 7 fits with an average of 36 data points and 10 variable parameters per fit and requiring an average of 11 iterations per fit took a total of 16 seconds of CPU time (exclusive of the plot step).

SKEWGAUS is operable on the IBM 360/370 computers. It was designed to fit into 128 K bytes (32 K words) of main core storage. Alternatively, the MCA data array may be placed in bulk (LCS) core storage to reduce the main core size to 96 K bytes.

A Fortran IV compiler is required.
10. REFERENCE

11. CONTENTS OF CODE PACKAGE
   Included are the referenced document and a reel of magnetic tape which contains the source code input written in Fortran IV and PL/1; total records 1383.

12. DATE OF ABSTRACT
    March 1984.

   KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
RSICC CODE PACKAGE PSR-164

1. NAME AND TITLE
   **TPASS:** A Gamma-Ray Spectral Data-Reduction and Analysis Code System.

2. CONTRIBUTOR
   Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; PDP-10.

4. NATURE OF PROBLEM SOLVED
   TPASS is a collection of routines designed to assist data reduction of gamma-ray spectra obtained with a high-resolution detection system. It is intended to be used as a research tool to speed up data reduction and to present data in a manner which allows the researcher to determine the adequacy of the analysis.

5. METHOD OF SOLUTION
   Using TPASS enables peaks in the spectrum to be identified, areas to be determined and corrected for detection efficiencies, and source identifications to be made, when possible, by comparisons with tabulated radionuclide decay data. Uncertainties assigned to peak area extractions are not derived from a “statistical” calculation but are determined from the estimated minimum continuum subtraction.

   TPASS uses a direct comparison of $E_{\text{gamma}}$ of the extracted data with tabulated values to indicate likely responsible radionuclides.

6. RESTRICTIONS OR LIMITATIONS
   Up to 20 gamma-ray energies and branching ratios may be used for each identified radionuclide. The number of radionuclides is limited only by the contents of the data library which is used.

7. TYPICAL RUNNING TIME
   No study has been made by RSICC of typical running times for TPASS.

8. COMPUTER HARDWARE REQUIREMENTS
   TPASS is operable on the PDP-10 computers.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.

10. REFERENCES

11. CONTENTS OF CODE PACKAGE
   Included are the referenced documents and a reel of magnetic tape which contains the source
code and sample problem input written in EBCDIC card images, plus output from the sample problem written in list format; total records 3811.

12. DATE OF ABSTRACT
April 1984.

KEYWORD: GAMMA-RAY SPECTRUM ANALYSIS
SECTION 3
UNFOLDING ANALYSIS CODES

These are programs designed to analyze gamma-ray pulse-height spectra obtained with a low-resolution detector, such as NaI or an organic scintillator. In most applications, the photon energy resolution is insufficient to resolve contributions to the measured spectra from photons having moderately different energies. These contributions would easily be identified in high-resolution Ge-detector data. This loss of resolution is usually compensated for by a substantial increase in efficiency.

Comments and assessments: as noted in the previous section, the computer codes usually evolve from some programmatic goal, involving a specific computer environment and/or a specific programming language. The compilers note that the quality of results is likely to be very dependent upon the adequacy of the user-supplied response matrix.
1. NAME AND TITLE
   **ALPHA-M**: Least-Squares Resolution of Gamma-Ray Spectra in Environmental Samples.

2. CONTRIBUTOR
   Tennessee Valley Authority, Muscle Shoals, Alabama.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; IBM 360/370.

4. NATURE OF PROBLEM SOLVED
   ALPHA-M is a standard least-squares computer program for analyzing gamma-ray spectral data obtained with NaI(Tl) scintillation detectors. This version of ALPHA-M has been prepared and tested to determine its capabilities and limitations for environmental monitoring. Either GEN4 or GENSTD is used to create standard libraries for ALPHA-M, and SIMSPEC is used to simulate spectra for ALPHA-M analysis.

5. METHOD OF SOLUTION
   ALPHA-M determines the activities of radioisotopes by a weighted least-squares resolution of their gamma-ray spectra. The application of the least-squares method to gamma spectral data yields superior quantitative results as compared with any other commonly used technique:
   1. Rapid data processing is possible.
   2. Spectra with large statistical variations in counting can be handled.
   3. The total spectrum, rather than just the photopeak regions, is used.
   4. Spectra with superimposed peaks can be analyzed.
   5. The standard error of the nuclide activity can be estimated.

6. RESTRICTIONS OR LIMITATIONS
   Many gamma-ray emitting radionuclides can be quantified at activity levels of about 10 pico-Curies per liter or less, depending on counting time, at a confidence level of 95 percent.

7. TYPICAL RUNNING TIME
   The sample problem input is a set of 3.5 liter water standards including 16 individual standard spectra for each of four 4" by 4" solid NaI crystals. The nuclide spectra are background stripped and the average background is an average of ten 4000-second backgrounds. The unit 5 input consists of a typical 3.5 liter water background spectrum and the spectrum from a 3.5 liter water cross-check from EPA. This problem took 7.73 cpu seconds on the IBM 370/3033.

8. COMPUTER HARDWARE REQUIREMENTS
   On the IBM 370/3033 the sample problem required 196 K in the GO step.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler and an Assembler language compiler are required.

10. REFERENCE
11. CONTENTS OF CODE PACKAGE
   Included are the referenced document and a reel of magnetic tape which contains the source code
   and sample problem input written in EBCDIC card images, plus output from the sample problem;
   total records 8154.

12. DATE OF ABSTRACT
   January 1982.

   KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS
1. NAME AND TITLE
   **CONFOLD:** Least-Structure Unfolding Code System for Measured Neutron and Gamma-Ray Spectra.

2. CONTRIBUTOR
   Los Alamos National Laboratory, Los Alamos, New Mexico.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; CDC 6600 (A), IBM 360/370 (B).

4. NATURE OF PROBLEM SOLVED
   CONFOLD solves integral equations of the first kind, subject to constraints on the structure of the solution.

5. METHOD OF SOLUTION
   CONFOLD unfolds smooth, continuous spectra using a method called "least structure analysis."

6. RESTRICTIONS OR LIMITATIONS
   It is necessary to use the correct uncertainties for the data and to use accurate response functions. Because no provision is made for including uncertainties in the response functions, it is important to determine how such uncertainties affect the unfolding and then to include them in the uncertainties assigned to the data.

7. TYPICAL RUNNING TIME
   CONFOLD runs in a few seconds on the CDC 6600 computer.

8. COMPUTER HARDWARE REQUIREMENTS
   CONFOLD is operable on the CDC 6600 computer. It requires about 13,000 words of storage for cases with 156 pulse-height channels and 21 response functions.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV and Assembler language compiler is required.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and a reel of magnetic tape which contains the source code and sample problem input written in BCD/EBCDIC card images, plus output from the sample problem written in list format; total records 710 (A) and 918 (B).

12. DATE OF ABSTRACT

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
1. **NAME AND TITLE**
   **CUPED:** Scintillation Spectrometer Polyenergetic Gamma Photon Experimental Distributions Unfolding Code.

   CUPED is a much modified version of CUBED.

2. **CONTRIBUTOR**
   NUS Corporation, Rockville, Maryland.

3. **CODING LANGUAGE AND COMPUTER**
   Fortran IV; IBM 360/75/91.

4. **NATURE OF PROBLEM SOLVED**
   CUPED unfolds sodium-iodide (thallium-activated) scintillation spectrometer polyenergetic gamma photon experimental distributions. It is designed to analyze the combination bremsstrahlung and monoenergetic gamma radiation field of cylindrical radioisotope power generators.

5. **METHOD OF SOLUTION**
   CUPED generates the detector system response matrix function and applies it to the monoenergetic spectral components discretely and to the bremsstrahlung iteratively. It corrects for iodine K X-ray escape, detector non-linearity, system drift, source decay, background, and detection efficiency. Results are presented in digital form for differential and integrated photon number and energy distributions and exposure dose.

   The standard spectra are normalized with respect to photopeak pulse-height and area and their photopeaks subtracted to obtain normalized Compton continua. The response matrix vectors are determined at each energy by interpolating the normalized continua and computing the associated Gaussian photopeaks. The thus interpolated vectors are redistributed in pulse-height to correspond to the detector system energy response and to satisfy the requirements of the spectra to be unfolded. Quadratic interpolation of the normalized continua is carried out either directly for gamma photon energies < 0.6616 MeV or by a method of parts, described in this report, for energies > 0.6616 MeV.

6. **RESTRICTIONS OR LIMITATIONS**
   None noted.

7. **TYPICAL RUNNING TIME**
   No study has been made by RSICC of typical running times for CUPED.

8. **COMPUTER HARDWARE REQUIREMENTS**
   CUPED is operable on the IBM 360/75/91 computers.

9. **COMPUTER SOFTWARE REQUIREMENTS**
   A Fortran IV compiler is required.
10. REFERENCES

11. CONTENTS OF CODE PACKAGE
Included are the referenced documents and a reel of magnetic tape which contains the source code and sample problem input written in BCD/EBCDIC card images, plus output from the sample problem written in list format; total records 5014.

12. DATE OF ABSTRACT
November 1983.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
1. NAME AND TITLE
   DOMUS: A Program for Decomposing A Two-Dimensional Spectrum

2. CONTRIBUTOR
   Joint Institute of Nuclear Research, Dubna, USSR, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; IBM PC/XT; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED
   DOMUS was written for the purpose of decomposing a two-dimensional spectrum into its components. DOMUS is a two-dimensional version of UPEAK (PSR-300).

5. METHOD OF SOLUTION
   The spectrum of nuclear reactions may be formally considered as a linear combination: \( s(x,y) = \sum (f_i(x,y), i=1,n) + b(x,y) + e(x,y); \) where \( f_i(x,y) \) is the \( i \)-th component of interest, \( b(x,y) \) is the background and \( e(x,y) \) is the statistical error with zero-valued mean and variance \( d(x,y) \); \( s(x,y) \) is the spectrum in two dimensions. Each measured component is regarded as a result of a transformation of its model \( m(x,y) \). The background is described by a second order surface. The method of least squares is used to determine the parameters in the equation.

6. RESTRICTIONS OR LIMITATIONS
   A maximum of 12 peaks in the spectrum interval can be used.

7. TYPICAL RUNNING TIME
   At the NEA Data Bank, the sample problem took about 5 minutes on an IBM PC/AT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS
   IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code was written in Fortran 77 and uses RM Fortran Version 2.42 or higher compiler. The PLINK86 overlay linker is also necessary.

10. REFERENCE
    “The Long Write Up of the Program FIND2+DOMUS,” informal notes by V. B. Zlokazov, JINR, Dubna, USSR.

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and one DS/HD (1.2 MB) 5.25 inch diskette.

12. DATE OF ABSTRACT
KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE; MICROCOMPUTER
1. **NAME AND TITLE**
   
   **FERDO/FERD:** Multichannel Neutron and Gamma-Ray Spectrum Matrix Unfolding Code Systems.

2. **CONTRIBUTOR**
   
   Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. **CODING LANGUAGE AND COMPUTER**
   
   Fortran IV; IBM 3033.

4. **NATURE OF PROBLEM SOLVED**
   
   FERDO and FERD solve the integral equation which relates a measured pulse-height distribution and associated uncertainties to the true energy spectrum of the incident radiation.

5. **METHOD OF SOLUTION**
   
   FERDO uses the method of constrained least-squares and biased estimation to solve a discretized representation of the integral unfolding problem and to compute a 2-sigma confidence interval for the true energy spectrum. FERD improves the FERDO solution by iteratively modifying the biased estimator.

6. **RESTRICTIONS OR LIMITATIONS**
   
   FERDO/FERD require accurate estimations of the actual detector response and the idealized detector response (normally the detector energy resolution). In-core memory requirements are roughly three times the size of the response matrix (number of rows times the number of columns) for FERDO and four times the size of the response matrix for FERD. Additionally, a scratch storage device must be specified for both FERDO and FERD.

7. **TYPICAL RUNNING TIME**
   
   Running time depends most strongly on the size of the response matrix. An 87 x 88 matrix problem required 4.5 s of IBM 3033 CPU time for FERDO and 15.2 s for FERD.

8. **COMPUTER HARDWARE REQUIREMENTS**
   
   FERDO/FERD is operable on the IBM 3033 computer.

9. **COMPUTER SOFTWARE REQUIREMENT**
   
   FERDO/FERD uses the proprietary DISSPLA graphics software package available from ISSCO, San Diego, California. It has been successfully run on the IBM 3033 computer under control of the MVS-JES2 Operating System. A Fortran IV compiler is required.

10. **REFERENCE**

11. CONTENTS OF CODE PACKAGE
   Included are the referenced document and a reel of magnetic tape which contains the source code
   and sample problem input written in EBCDIC card images, plus output from the sample problem; total
   records 5,332.

12. DATE OF ABSTRACT
   October 1983.

   KEYWORDS: UNFOLDING; GAMMA-RAY SPECTRUM ANALYSIS
1. NAME AND TITLE


2. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

Fortran 77 and Basic; IBM PC and compatibles.

4. NATURE OF PROBLEM SOLVED

FERD-PC solves the integral equation which relates a measured pulse-height distribution and associated uncertainties to the true energy spectrum of the incident radiation. FERD-PC is a modified version of FERD, which is included in PSR-102. Several changes were made to include an interactive binning code, a flux integration code, and a plotting utility.

5. METHOD OF SOLUTION

The FERD method uses constrained least-squares and biased estimation to solve a discretized representation of the integral unfolding problem and to compute a 2-sigma confidence interval for the true energy spectrum. The mathematical method of FERD-PC differs from FERD only in that FERD-PC assumes no uncertainty in the response matrix, while FERD allows additional uncertainty by means of an upper and lower response matrix.

6. RESTRICTIONS OR LIMITATIONS

FERD requires an accurate estimation of the actual detector response and the idealized detector response (detector resolution). The limit on the size of the response is highly dependent on available computer memory. A 68 x 55 response matrix requires a minimum of 360 kilobytes of computer memory.

7. TYPICAL RUNNING TIME

Running time depends most strongly on the size of the response matrix and the number of output files it generates. The sample problem used 212 seconds on an IBM PC/XT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS

FERD is operable on IBM PC or compatibles running DOS version 2.1 or later. A minimum of 360 K of available user memory is required, and a math coprocessor must be installed. FERD-PC has been run on DEC VAX II and IBM PS/2 computers. PLOTFERD requires a HP 7475A or equivalent plotter.

9. COMPUTER SOFTWARE REQUIREMENT

FERD-PC uses the Microsoft Fortran (Version 4.01) compiler, and the Microsoft Quickbasic
compiler was used for PLOTFERD.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and one double-sided, double density (360 K) diskette containing the source code and sample problem input, plus output from the sample problem.

12. DATE OF ABSTRACT
    June 1989.

    KEYWORDS UNFOLDING; GAMMA-RAY SPECTRUM ANALYSIS
1. NAME AND TITLE
   **NAISAP**: Theory and Use of Gamma-Ray Spectrum Analysis Codes for NaI(Tl) Detectors.

2. CONTRIBUTOR
   Japan Atomic Energy Research Institute, Tokai Research Establishment, Ibaraki-Ken, Japan.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; FACOM 230-60.

4. NATURE OF PROBLEM SOLVED
   NAISAP analyzes the NaI(Tl) gamma-ray spectrum and other types of spectra to determine the energies and intensities of the peaks detected. The spectrum is plotted in option.

5. METHOD OF SOLUTION
   The analysis is carried out by the photopeak method on the basis of the NaI(Tl) response function represented in an analytical form. The peak search is based on the first derivative method accompanied with various peak shape tests. The usual least squares method is adopted for resolving the complex of peaks. Values of the parameters for constructing the NaI(Tl) response are stored as data for two detector sizes: 1-3/4" phi x 2" and 3" phi x 3."

6. RESTRICTIONS OR LIMITATIONS
   NAISAP accepts a spectrum of a maximum of 1024 channels with up to 49 peaks. Response functions of detectors with dimensions different from those mentioned above must be given by the user in specifying the parameters as functions of the photon energy.

7. TYPICAL RUNNING TIME
   NAISAP requires approximately one second for the analysis of each peak.

8. COMPUTER HARDWARE REQUIREMENTS
   NAISAP is operable on the FACOM 230-60 computer. A 76 K word memory is required. A CALCOMP plotter is optional.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.

10. REFERENCES
11. CONTENTS OF CODE PACKAGE
   Included are the referenced documents and a reel of magnetic tape which contains the source code
   and sample problem input written in EBCDIC card images, plus output from the sample problem; total
   records 3927.

12. DATE OF ABSTRACT
   March 1984.

   KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; UNFOLDING
NEA CODE PACKAGE NEA 0487

NEA 0487 RADAK,MULTICHANNEL_ANALYSER N_SPECTRA & GAMMA_SPECTRA UNFOLDING 810619

1. NAME OR DESIGNATION OF PROGRAM. RADAK.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
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<tr>
<td>RADAK</td>
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<td>RADAK</td>
<td>NEA 0487/02</td>
<td>IBM 370 series</td>
<td>IBM 370 series</td>
<td>T</td>
</tr>
</tbody>
</table>

3. NATURE OF PHYSICAL PROBLEM SOLVED.

RADAK unfolds flux spectra from the output of multi-channel and single-channel neutron or gamma ray detectors. The errors, including correlations, of the flux solution are estimated.

4. METHOD OF SOLUTION.

The solution is determined which maximises the likelihood of the observed measurements subject to the fluxes remaining positive. The errors are estimated using Monte Carlo, by taking random samples about the measurements.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.

Maximum number of -
- spectra unfolded simultaneously - 10
- detector channels - 200
- flux groups - 60

6. TYPICAL RUNNING TIME.

3 minutes CPU for unfolding (with error analysis) the output from 5 proportional counters and 3 threshold detectors at 3 positions. 60 flux groups were used, and a total of 76 channels.

7. UNUSUAL FEATURES OF THE PROGRAM.

The output from several multi-channel and single-channel detectors may be analysed simultaneously to produce a single-valued flux solution. Allowance may be made for the uncertainties in the detector response functions.
8. RELATED AND AUXILIARY PROGRAMS.

The program package also contains two auxiliary programs, PRC and NE213, which generate response matrices respectively for gas-filled spherical proportional counters and NE213 organic liquid scintillation spectrometers. The NE213 program may also be used for grouping or differentiating the counts from any type of spectrometer in preparation for input to RADAK. Several routines from the Harwell subroutine library are included.

9. STATUS

NEA 0487/01 : Arrived at NEADB
              : in preparation
              : Tested at NEADB
NEA 0487/02 : Arrived at NEADB
              : in preparation
              : Tested at NEADB

10. REFERENCES.

NEA 0487/01 :
- J. Patry: Three Programs for the Calculation of Flux Spectra from the Output of Neutron or Gamma-ray Detectors: PRC, NE213 and RADAKA TM-RZ-58/2 (December 7, 1978)
NEA 0487/02 :

11. MACHINE REQUIREMENTS.

The program requires 350 kbytes of code storage.

12. PROGRAMMING LANGUAGE USED

NEA 0487/01 : FORTRAN+ASSEMBLER
NEA 0487/02 : FORTRAN+ASSEMBLER

13. OPERATING SYSTEM OR MONITOR UNDER WHICH PROGRAM IS EXECUTED.

IBM 370 O.S. MVS.

14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.
15. NAME AND ESTABLISHMENT OF AUTHOR.

Mr. M.J. Grimstone
UKAEA
Atomic Energy Establishment
Winfirth
Dorchester, Dorset
United Kingdom.

16. MATERIAL AVAILABLE

NEA 0487/01:
Report: AEEW-M1483 (July 1977)
Report: AEEW-M1455 (December 1976)
SOURCE (F4, ASSEMBLER) 2541 records
SAMPLE INPUT DATA 723 records
SAMPLE OUTPUT 2190 records
PRC (CAL. OF RESPONSE MATRIX FOR RADAK) 1232 records
SAMPLE INPUT FOR PRC 46 records
SAMPLE OUTPUT OF PRC 237 records
NE213 (PREPARATION OF RESPONSE MATRIX) 1042 records
SAMPLE INPUT FOR NE213 22 records
SAMPLE OUTPUT OF NE213 848 records
FEHLIM (COMPUTATION OF ERROR FUNCTION) 13 records

NEA 0487/02:
Report: AEEW-M1483 (July 1977)
Report: AEEW-M1455 (December 1976)
INFORMATION 2 records
PRC ASSEMBLER ROUTINES 75 records
PRC F4 SOURCE EBCDIC 1782 records
PRC SAMPLE PROBLEM INPUT 14 records
PRC SAMPLE PROBLEM OUTPUT 764 records
NE213 ASSEMBLER ROUTINES 161 records
NE213 F4 SOURCE EBCDIC 1883 records
NE213 SAMPLE PROBLEM INPUT 41 records
NE213 SAMPLE PROBLEM OUTPUT 183 records
RADAK ASSEMBLER ROUTINES 267 records
RADAK F4 SOURCE EBCDIC 3239 records
RADAK SAMPLE PROBLEM INPUT 624 records
RADAK SAMPLE PROBLEM OUTPUT 6331 records
JCL AND INFORMATION 100 records

17. CATEGORY = 0,

KEYWORDS Monte Carlo method
gamma spectra
multi-channel analysers
neutron detectors
neutron flux
neutron spectra
spectra unfolding
spectrometers
1. NAME OR DESIGNATION OF PROGRAM - UNSPEC (Unfolding X-Ray Spectrums).

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
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<td>ESTS0827/01</td>
<td>CRAY 1</td>
<td>CRAY 1</td>
<td>A</td>
</tr>
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</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

UNSPEC is used to solve the problem of unfolding an observed X-ray spectrum given the response matrix of the measuring system and the measured signal valued.

4. METHOD OF SOLUTION

UNSPEC uses an iterative technique to solve the unfold problem. Qualitatively, the solution proceeds as follows: 1. Choose a trial spectrum consistent with the experiments criterion for smoothness, 2. Fold this spectrum with the known response matrix, 3. Compare the measured and calculated signal values, 4. Adjust the trial spectrum in order to improve the agreement between the measured and calculated signal values, 5. Repeat steps 1-4 until the final result is consistent with the measured signal values to some arbitrary criterion selected by the experimenter.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

6. TYPICAL RUNNING TIME

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

ESTS0827/01 : Known to NEADB
             : Requested by NEADB
             : Arrived at NEADB

10. REFERENCES

ESTS0827/01 :
    - H.F. Finn:
      UNSPEC Reference Manual version 10/29/82
      UCID-19616 (December 1, 1982)
11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

ESTS0827/01 : LLNL-FORTRAN

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

Machine dependent.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

H.F. Finn
Lawrence Livermore National Lab., CA (United States)

16. MATERIAL AVAILABLE

ESTS0827/01 :
UNSPEC.SUB Source code
UNSPEC.CAR Sample problem (cards)
UNSPEC.SOC Sample problem (sock)
Report: UCID-19616 (December 1, 1982)

17. CATEGORY = O , W ,

KEYWORDS
gamma detectors
radiation detectors
spectra unfolding
x-rays
1. NAME AND TITLE
   **UPEAK**: A Program for Decomposing A One-Dimensional Spectrum

2. CONTRIBUTOR
   Joint Institute of Nuclear Research, Dubna, USSR, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; IBM PC/XT; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED
   **UPEAK** was written for the purpose of decomposing a one-dimensional spectrum into its components.

5. METHOD OF SOLUTION
   The spectrum of nuclear reactions may be formally considered as a linear combination: \( s(x) = \sum_{i=1}^{n} (f_i(x) + b(x) + e(x)) \); where \( f_i(x) \) is the i-th component of interest, \( b(x) \) is the background and \( e(x) \) is the statistical error with zero-valued mean and variance \( d(x) \); \( s(x) \) is the spectrum. Each measured component is regarded as a result of a transformation of its model \( m(x) \). Regression analysis is used to determine the least squares estimates of some of the parameters.

6. RESTRICTIONS OR LIMITATIONS
   A maximum of 20 components in the spectrum interval can be used.

7. TYPICAL RUNNING TIME
   At the NEA Data Bank, the sample problem took about 4 minutes on an IBM PC/AT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS
   IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code was written in Fortran 77 and uses RM Fortran Version 2.42 or higher compiler. The PLINK86 overlay linker is also necessary.

10. REFERENCES
    “The Long Write Up of the Program UPEAK,” informal notes by V. B. Zlokazov, JINR, Dubna, USSR.

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and one DS/HD (1.2 MG) 5.25 inch diskette.

12. DATE OF ABSTRACT
KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; INTERACTIVE, ON-LINE; MICROCOMPUTER
SECTION 4
MODEL PREDICTIONS OF PHOTON YIELDS

In this section are listed programs to predict photon yields. These computer codes are all based on compound-nucleus/statistical model formalisms; they also indicate that photon production is included in the calculations.

Programs of the inventory type, for example ORIGEN¹, are not listed in this compilation. However, in the next section is listed the program GABAS which can be used to interface with the output of an inventory code to calculate time-dependent photon spectra.

Also, we do not list Optical-Model analysis programs or other programs using direct-interaction calculations. The underlying theories for these programs are designed to predict angular distributions of outgoing nucleons or heavy ions and not for photon production.

It should be noted that the Information Centers have other programs of the statistical-model/compound-nucleus type but which do not indicate photon-production computations in the abstracts of the programs. Some of these other programs are:

CEM95 RSICC Code Package PSR-357; NEA Code Package IAEA1247;
COMNUC3B RSICC Code Package PSR-302
HAUSER*5 RSICC Code Package PSR-152
NX1-NX2 RSICC Code Package PSR-310; NEA Code Packages IAEA0918 and IAEA0919;
PREANG RSICC Code Package PSR-166
PREM RSICC Code Package PSR-224; NEA Code Package NEA 0888;
SPECTER RSICC Code Package PSR-023
STAPRE-H RSICC Code Package PSR-325;

REFERENCE

1. NAME AND TITLE
   ALICE-91: Statistical Model Code System with Fission Competition.
   ALICE-87: Revised ALICE for Personal Computer.
   ALISO-PC: Gives Isotopically Weighted Results.

2. CONTRIBUTORS
   Lawrence Livermore National Laboratory, Livermore, California.
   International Atomic Energy Agency, Vienna, Austria, through the Nuclear Energy Agency Data Bank, Gif-sur-Yvette, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; Cray XMP (PO0146CYOMP00), IBM PC (P00146IPCAT00), SUN (P00146SUN0401).

4. NATURE OF PROBLEM SOLVED
   Several types of calculations and combinations can be performed including a standard Weisskopf-Ewing evaporation with multiple particle emission, s-wave approximation to give an upper limit to the enhancement of gamma-ray deexcitation due to angular momentum effects, and an evaporation calculation that can include fission competition via the Bohr-Wheeler approach. ALICE91 calculates precompound decay via Hybrid and GDH models with multiple precompound decay algorithms, single and double differential spectra, and reaction product cross sections.

5. METHOD OF SOLUTION
   ALICE/85/300 and later revisions of the ALICE/LIVERMORE 82 computer code do precompound, compound/statistical fission calculations in the general framework of the Weisskopf-Ewing evaporation model, the Bohr-Wheeler transition state model for fission, and the hybrid/geometry dependent models for precompound decay. ALICE/85/300 allows a variable energy mesh size, excitation energies up to 300 MeV, and incorporates several other improvements in calculational approaches.
   ALICE91 includes options for shell dependent level densities, and an option to use systematics for angular distribution. The new version also includes gamma-ray competition with particle decay modes.
   The IBM PC version (B) was converted from mainframe ALICE-87, which is a revision of ALICE/85/300. Input default options were included in this version. Refer to comments in the file ALICE1.FOR for information on modifications. ALISO differs only in that it will do calculations for natural isotopic targets, giving weighted results at the end.
   The Sun version was converted from ALICE-91 that was released in April, 1991. This version differs from earlier releases in the following ways: 1) Level density options due to Katoria/Ramamurthg may be selected.; 2) Level density options due to Ignatyuk may be selected.; 3) The systematics expressions for precompound angular distributions of C. Kalbach are an option. (These are faster than the option based on n-n scattering kinematics and agree more with experimental results.); 4) Gamma-ray spectra are given for the reactions, and gamma rays compete with nucleon emission (Mitigates problems with trapped protons for very proton rich nuclei.; 5) This version may be used to calculate for isotopically mixed targets (e.g. natural isotopic composition).

6. RESTRICTIONS OR LIMITATIONS
   Users must refer to comments in the Fortran source files for input instructions and information. If running the PC version on 32-bit word-length machines, remove CXXXXX from double precision
7. **TYPICAL RUNNING TIME**

The sample input took about 6 seconds of CPU time on the Cray XMP under UNICOS. The sample case for ALICE-87 took 23 minutes on an IBM PC/XT running at 4.7 megahertz with a math co-processor. The ALISO case took 4 minutes on the same computer.

8. **COMPUTER HARDWARE REQUIREMENTS**

Version A is operational on the Cray XMP, and Version B has run on both IBM PC/XT and /AT computers with math co-processors. Memory requirements for the executable modules on an IBM PC/AT are: 530 K (ALICE) and 525 K (ALISO). Version C is operational on Sun workstations.

9. **COMPUTER SOFTWARE REQUIREMENTS**

The Cray/CTSS version used the CIVIC compiler and the Cray/UNICOS version used the CFT77 compiler. For ALICE-87 IBM Professional Fortran Version 1.0 was used, and for ALISO, Microsoft's Fortran 4.01 was used. The Sun version was tested with the SC1.0 f77 compiler. The code was tested on a Sun SPARCstation SLC under-SunOS 4.1.1 using SUN FORTRAN v1.4. The code was also tested on a Sun SPARCstation 2 under SOLARIS 2.3 (Sun 5.3) using SUN FORTRAN 2.0.

10. **REFERENCES**

a. **Included in the documentation:**

   R. Roussin, Informal Input Instructions for ALICE/85/300 (February 1987).

b. **Background information:**

   M. Blann, W. Scobel, and E. Plechaty, “Precompound Nucleon Angular Distributions in the

11. CONTENTS OF CODE PACKAGE
Included are the referenced documents (a), the ALICE-91 source code, sample input and output for version A. Version B includes both the ALICE-87 and ALISO codes. Each package is available on one DS/HD (1.2MB) diskette in DOS format. The SUN version is alternately available on one DS/HD (1.44MB) diskette in UNIX tar format.

12. DATE OF ABSTRACT

**KEYWORDS:** NUCLEAR MODELS; WORKSTATION; MICROCOMPUTER
1. NAME AND TITLE

CASTHY: Statistical Model Calculation for Neutron Cross Sections and Capture Gamma-Ray Spectra.

2. CONTRIBUTOR

Japan Atomic Energy Research Institute, Tokai-mura, Japan.

3. CODING LANGUAGE AND COMPUTER/OPERATING SYSTEM

Fortran 77, FACOM computers and IBM RISC 6000.

4. NATURE OF PROBLEM SOLVED

This code has been utilized as a tool for nuclear data evaluations. It is used to calculate neutron cross sections of total, shape elastic scattering and compound nucleus formation with the optical model, and compound elastic scattering, inelastic scattering and capture cross sections by the statistical model applying Hauser-Feshbach and/or Moldauer formula. The other cross sections such as the \((n,2n)\), \((n,p)\), \((n,t)\) reactions are treated as cross sections of competing processes, and their sum is given through input data. This code calculates also capture gamma-ray spectra. Branching ratio for primary transition can be treated in a particular way, if necessary.

5. METHOD OF SOLUTION

The total transmission coefficient is modified so that the total reaction cross section obtained by using the optical model may be conserved. The transmission coefficients for neutrons and gamma-rays are rewritten by considering an effect of \((n,\gamma-n')\) process.

6. RESTRICTIONS OR LIMITATIONS

For the normalization of cross section, the normalization energy point should be included in the incident energy points of input data. Some other limitations exist depending on options.

7. TYPICAL RUNNING TIME

On an IBM RISC system 550, sample problems 1, 2, and 3 took 14.6, 15.8 and 86.9 seconds respectively.

8. COMPUTER HARDWARE REQUIREMENTS

The code was developed on the FACOM computers and tested on the IBM RISC 6000.

9. COMPUTER SOFTWARE REQUIREMENTS

The code was written in Fortran 77 and tested using the xlf Fortran compiler under the AIX 3.1 operating system on the IBM RISC 6000.

10. REFERENCE


11. CONTENTS OF CODE PACKAGE

Included are the referenced document and one DS/HD (1.2MB) 5.25-in. diskette which includes the source files, sample input and output.
KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; NEUTRON; NUCLEAR MODELS; PARAMETRIC MODELS
1. NAME AND TITLE
   **EMPIRE**: A Pre-equilibrium Compound Nuclear Model Code For Personal Computers

2. CONTRIBUTOR
   Institute of Nuclear Studies, Warsaw, Poland through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED
   EMPIRE calculates spectra and cross sections for capture and/or multistep nuclear reactions in the frame of a combined pre-equilibrium and compound nucleus mechanism model.

5. METHOD OF SOLUTION
   Angular momentum conservation is observed throughout the whole calculation. The decay of the compound nucleus is treated either in terms of the HRTW theory, to account for the width fluctuation effects, or in terms of standard Hauser-Feshbach theory if many open particle channels cause the fluctuations to cancel. The transmission coefficients of the nuclear potential are calculated with an optical model subroutine. The full gamma cascade is included in the calculations providing the gamma spectra and populations of the discrete levels in the residual nuclei.

6. RESTRICTIONS OR LIMITATIONS
   The particles considered in the code are neutrons, protons and alphas. The energy discretization of the continuum is confined to 120 points. The maximum number of partial waves is 30.

7. TYPICAL RUNNING TIME
   The sample input problems (test cases 1 and 2) were run at NEA Data Bank on an IBM PC/AT with a math coprocessor. With the PROFORT compiler, problem 1 took 15 minutes, 8 seconds; problem 2 took 32 minutes, 3 seconds. With the RM/Fortran compiler, problems 1 and 2 took 8 minutes, 48 seconds and 21 minutes, 55 seconds respectively.

8. COMPUTER HARDWARE REQUIREMENTS
   EMPIRE runs on an IBM PC/AT with a math coprocessor.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code was written in Fortran 77. The NEA Data Bank used IBM Professional Fortran version 1.0 and the RM/Fortran compiler, version 2.42 under the MS-DOS 3.20 operating system.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and one DS/HD (1.2 MB) 5.25-inch diskette.
12. DATE OF ABSTRACT
November 1990.

KEYWORDS: MICROCOMPUTER; NUCLEAR MODELS; NEUTRON; PROTON
1. **NAME AND TITLE**
   **ERINNI:** Optical Model Calculation of Multiple Cascading Particle Emissions.

2. **CONTRIBUTOR**
   Centro di Calcolo del CNEN, Bologna, Italy, through the NEA Data Bank, Gif-sur-Yvette, France.

3. **CODING LANGUAGE AND COMPUTER**
   Fortran IV; IBM 360/370.

4. **NATURE OF PROBLEM SOLVED**
   ERINNI offers an optical model calculation of multiple cascading particle emissions. It computes 42 cross sections for each incident energy representing all possible compound nucleus processes of types (x,a), (x,ab), and (x,abc) where x can be indifferently a neutron, proton, or alpha particle; a and b can be a neutron, a proton, an alpha or gamma particle; and c can be a neutron or a gamma particle. ERINNI is particularly useful for extensive cross section calculations such as those in the range of reactor calculation needs.

5. **METHOD OF SOLUTION**
   The scattering amplitudes and the other optical model quantities are calculated in accordance with spherical local potentials by the usual methods. Parameters are needed for 10 residual nuclei, hence particular care was devoted to reducing the input procedure. The table for pairing energies, the Mass excess table, the level density data systematics, and the optical model parameter sets most frequently used in literature are all incorporated in the program and can be used optionally as an alternative to more specific choices of data.

6. **RESTRICTIONS OR LIMITATIONS**
   No width fluctuation is included because it is devised for high energy calculations.

7. **TYPICAL RUNNING TIME**
   The OECD NEA Data Bank executed the test case included in the package on an IBM 3084Q computer in 375 seconds of CPU time. Computing time was reduced because the various optical model transmission coefficients and consequent decay probabilities at a given incident energy, when they are calculated within appropriately narrow energy intervals, lend themselves to interpolation.

8. **COMPUTER HARDWARE REQUIREMENTS**
   ERINNI is operable on the IBM 360/370 computers. 240 kbytes of fast core memory is required if used together with the overlay structure.

9. **COMPUTER SOFTWARE REQUIREMENTS**
   A Fortran IV compiler is required.

10. **REFERENCE**
11. CONTENTS OF CODE PACKAGE
   Included are the referenced document and a reel of magnetic tape which contains the source code
   and sample problem input written in EBCDIC card images; total records 2914.

12. DATE OF ABSTRACT
   June 1986.

   KEYWORD: NUCLEAR MODELS
1. NAME AND TITLE
   EXIFON-GAMMA: A Model For Statistical Multistep Direct and Multistep Compound Reactions

2. CONTRIBUTOR
   Technische Universität Dresden, Germany, through NEA Data Bank, France.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; IBM PC/XT; IBM PC/AT.

4. NATURE OF PROBLEM SOLVED
   EXIFON-GAMMA predicts emission spectra for neutrons, protons, alphas, and photons including equilibrium, pre-equilibrium, direct as well as multiple particle emission processes.

5. METHOD OF SOLUTION
   The model is based on random matrix physics with the use of the Green's function formalism. All calculations are performed without any free parameters. Results are presented for bombarding energies below 30 MeV.

6. RESTRICTIONS OR LIMITATIONS
   None noted.

7. TYPICAL RUNNING TIME
   The sample problem (as listed in RUN.BAT, using the FE56 data) took about 50 seconds on an IBM PC/AT with a math co-processor.

8. COMPUTER HARDWARE REQUIREMENTS
   IBM PC and compatibles with math co-processor.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code was written in Fortran 77 and uses RM Fortran Version 2.42 or Microsoft Fortran Version 4.01.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and one DS/HD (1.2 MB) 5.25 inch diskette.

12. DATE OF ABSTRACT

   KEYWORDS: MICROCOMPUTER; NEUTRON; NUCLEAR MODELS; PROTON
1. NAME AND TITLE
   **GNASH-FKK:** Pre-equilibrium, Statistical Nuclear-Model Code System for Calculation of Cross Sections and Emission Spectra.

   **AUXILIARY CODE**
   SEARCH3: Operates on the output of the FKK-GNASH code to produce ENDF/B-formatted cross section records.

   **DATA LIBRARY**
   STRUCTURE.DAT: Nuclear level energies, spins, parities, and gamma-ray branching ratios.
   TRANS.COEF: Particle transmission coefficients from spherical or deformed optical model calculations.
   MASS.DAT: Table of ground-state masses, spins, and parities.

2. CONTRIBUTOR
   Los Alamos National Laboratory, Los Alamos, New Mexico.

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; Cray (P00125/CY000/02).

4. NATURE OF PROBLEM SOLVED
   GNASH provides a flexible method by which reaction and level cross sections, isomer ratios, and emission spectra (neutron, gamma-ray, and charged-particle) resulting from particle- and photon-induced reactions can be calculated. The September 1991 release of GNASH incorporated an additional option for calculating gamma-ray strength functions and transmission coefficients by including the Kopecky-Uhl model. In addition, improvements were made to the output routines, particularly regarding gamma-ray strength function information. Major improvements in the 1995 FKK-GNASH release include added capabilities: to read in externally calculated preequilibrium spectrum from, e.g., Feshbach-Kermin-Koonin theory, to do multiple preequilibrium calculations, to calculate appropriate spin distributions for nuclear states formed in preequilibrium reactions, and to do incident-photon calculations. Additional improvements are noted in the READ.ME file.

5. METHOD OF SOLUTION
   GNASH uses Hauser-Feshbach theory to calculate complicated sequences of reactions and includes a pre-equilibrium correction for binary tertiary channels. Gamma-ray competition is considered in detail for every decaying compound nucleus. A multi-humped fission barrier model is included for fission cross-section calculations. Three options for level densities are available.

6. RESTRICTIONS OR LIMITATIONS
   In its present configuration, each calculation can handle decay sequences involving up to 38 compound nuclei and each decaying compound nucleus can emit a maximum of 5 types of radiation (neutrons, gamma rays, protons, alphas, etc.). Angular-momentum effects and conservation of parity are included explicitly. Each residual nucleus in a calculation can contain up to 78 discrete levels whereas its continuum region can be represented by up to 204 energy bins. The incident-particle types that are permitted are neutrons, protons, deuterons, tritons, $^3$He, and $^4$He. Angular distributions are not
calculated; i.e., isotropy is assumed in the center-of-mass (c.m.) system. Angular distribution effects can be added in postprocessing utility codes making use of, for example, Kalbach-Mann systematics.

7. **TYPICAL RUNNING TIME**
   The running times typically range from a few seconds to a few minutes per incident energy depending upon incident particle energy, mass range of the target, number of compound nuclei included, and the energy bin width that is used.

8. **COMPUTER HARDWARE REQUIREMENTS**
   GNASH was developed originally on the CDC 6600 and 7600 computers and is now maintained on Cray. It requires 3,500,000 words of storage in its present configuration. Storage requirements may be reduced by changing the value of 'nkdim' and other parameters in a PARAMETER statement. The current value for nkdim is 204 energy bins.

9. **COMPUTER SOFTWARE REQUIREMENTS**
   The codes run on Cray computers under the UNICOS operating system. The gnash and search3 Fortran sources call routines which are Cray specific, but they can be ported to other Unix systems. Calls to filerep and qstart equate internal and external file names and may be removed. Substitutions need to be supplied for "date" and "second" which retrieve calendar data and time of day. Two "encode" statements in search3 may need to be changed.

10. **REFERENCES**
    a. included in documentation:
       P. G. Young, README (January 1996).
    b. background information:

11. **CONTENTS OF CODE PACKAGE**
    Included are the referenced documents and one 3.5-in. DS/HD (1.44 MB) diskette containing the source code, data libraries, sample problem input and output in either compressed tar or DOS format.

12. **DATE OF ABSTRACT**

**KEYWORD:** NUCLEAR MODELS
1. NAME AND TITLE

2. CONTRIBUTORS
Institute of Physics, Slovak Academy of Sciences, Bratislava, Czechoslovakia through the NEA Data Bank, Issy-les-Moulineaux, France.

3. CODING LANGUAGE AND COMPUTER
Fortran 77; IBM PC and compatibles.

4. NATURE OF PROBLEM SOLVED
PEGAS is a pre-equilibrium-equilibrium gamma-and-spin code, based on the unified model of nuclear reactions. Therein, the equilibrium (compound-nucleus) emission is treated as an organic part of the pre-equilibrium emission. The code has two important novel features: the angular-momentum couplings are correctly taken into account for all processes (equilibration, particle and gamma emission), and nucleon as well as gamma emissions are calculated with all possible cascades for all possible sequences of the ejectiles. PEGAS addresses the lack of possibilities, with currently existing codes, to trace a complete development of the reaction system including the consistent treatment of cascade emissions (e.g., the pre-equilibrium emission is often limited to the primary particle only). PEGAS also provides a full treatment of angular momentum conservation.

5. METHOD OF SOLUTION
Master equations of the exiton model are solved by the algorithm of Chatterjee and Gupta. Gamma emission is according to Oblozinsky. The general philosophy of the PEGAS code is derived from the nonspin version named PEQAG.

6. RESTRICTIONS OR LIMITATIONS
The present version of PEGAS is designed for reactions induced by nucleons, though other projectiles are allowed as well, leading to the composite system with the excitation energy not exceeding 30 MeV and with nuclear spins limited to $< 15\hbar$. The limitations in spin, energy, and number of successive nucleons may be shifted by adjusting the dimensions of the array.

7. TYPICAL RUNNING TIME
Sample problem execution time:
(on a Northgate 486/66) 9 minutes 43 seconds

8. COMPUTER HARDWARE REQUIREMENTS
PEGAS runs on an IBM PC or compatible with at least 578K of RAM (recommended) for compilation and linking and at least 520K for execution. Approximately 3.5 MB of free disk space is required for execution because the disk is used for temporary file swapping.

9. COMPUTER SOFTWARE REQUIREMENTS
PEGAS runs under DOS. The MS Fortran 5.0 compiler was used to create the executable included in the package.
10. **REFERENCE**

11. **CONTENTS OF CODE PACKAGE**
   Included are the referenced document and 1 DS/HD 5.25-in. (1.2 MB) diskette which contains the source code, executable, sample input/output, and a README.RSI file which describes the installation and operation of PEGAS.

12. **DATE OF ABSTRACT**
   September 1993.

**KEYWORDS:** NUCLEAR MODELS; MICROCOMPUTER
1. **NAME AND TITLE**
   **PEQAG-2:** A Pre-equilibrium Computer Code With Gamma Emission

2. **CONTRIBUTOR**
   Institute of Physics, Bratislava, Czechoslovakia, through IAEA, Vienna, through NEA Data Bank, France.

3. **CODING LANGUAGE AND COMPUTER**
   Fortran 77; IBM PC/AT.

4. **NATURE OF PROBLEM SOLVED**
   PEQAG-2 performs an exciton model calculation of angle-integrated nucleon and gamma energy spectra. All the emissions are treated consistently within the pre-equilibrium approach based on the master equations of the model. Multiple particle and/or multiple gamma emissions are included.

5. **METHOD OF SOLUTION**
   Angle-integrated energy spectra of neutrons, protons and gammas, as well as the corresponding integrals are computed. No angle-dependent or spin-dependent calculations are included. The state density used is the equidistant-spacing model in the finite potential well. Inverse cross sections may be supplied by the program according to the approximation of Chatterjee et al., and the GDR shape is also built-in.

6. **RESTRICTIONS OR LIMITATIONS**
   Up to four nucleons are emitted and interspersed and/or preceded by arbitrary number of gammas. The maximum energy is 100 times the energy step used.

7. **TYPICAL RUNNING TIME**
   The sample input problem was run at NEA Data Bank on an IBM PC/AT with a math coprocessor. The problem took 8 minutes and 50 seconds.

8. **COMPUTER HARDWARE REQUIREMENTS**
   PEQAG-2 runs on an IBM PC/AT with a math coprocessor.

9. **COMPUTER SOFTWARE REQUIREMENTS**
   The code was written in Fortran 77. The NEA Data Bank used Microsoft Fortran version 5.0 and the RM/Fortran compiler, version 2.42 under the MS-DOS 3.20 operating system.

10. **REFERENCE**

11. **CONTENTS OF CODE PACKAGE**
    Included are the referenced document and one DS/HD (1.2 MB) 5.25-inch diskette.

12. **DATE OF ABSTRACT**
    105
November 1990.

**KEYWORDS:** GAMMA RAY SOURCE ANALYSIS; MICROCOMPUTER; NUCLEAR MODELS; NEUTRON; PROTON
1. NAME AND TITLE

TNG1: A Multistep Statistical Model Based on the Hauser-Feshbach Theory For The Evaluation Of Neutron Data.

2. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

Fortran 77; VAX 6000.

4. NATURE OF PROBLEM SOLVED

The TNG1 code is a multistep statistical model based on the Hauser-Feshbach theory including width-fluctuation corrections and pre-compound effects. Statistical model calculations are frequently performed for medium and heavy nuclei.

5. METHOD OF SOLUTION

The Hauser-Feshbach part of the TNG1 code is multi-step, but angular distribution can be calculated only for the binary step. The pre-compound portion is single step, in this case angular distribution is calculated on the basis of partial wave interference (partial relaxation of the random phase approximation in the H-F formalism). Quantities calculated include: elastic, total, inelastic, \((n,g)\), \((n,n')\), \((n,p)\), \((n,a)\), \((n,f)\), \((n,2n)\), \((n,np)\), \((n,na)\), \((n,nf)\),\(\ldots\), secondary particle and gamma ray production spectra, angular distributions of the first outgoing particles, and the production cross sections of isomeric states.

6. RESTRICTIONS OR LIMITATIONS

\((n,gx)\) has not been included. Dimensions of the transmission coefficients are such that cross sections can be calculated up to 40 MeV for Ca-40 and 20 MeV for Pu-242. The maximum number of discrete levels is 40, the number of continuum bins is limited to 40 for each residual nuclide, and the number of outgoing particles is limited to 3.

7. TYPICAL RUNNING TIME

On an the VAX 6000, sample problem 1 took about 2 minutes of CPU time (wall clock time).

8. COMPUTER HARDWARE REQUIREMENTS

TNG1 runs on the VAX family of computers.

9. COMPUTER SOFTWARE REQUIREMENTS

A Fortran 77 compiler is required. The code was compiled with VAX/Fortran on the VAX 6000 under the VAX/VMS operating system.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
   Included are the referenced documents and one DS/DD 5.25-inch diskette (360 K) which contains the source code and sample problem input and output.

12. DATE OF ABSTRACT

   KEYWORDS: EXPERIMENTAL DATA ANALYSIS; NEUTRON; NUCLEAR MODELS
SECTION 5
MISCELLANEOUS PROGRAMS

This section contains computer codes of interest and application to photon data which are not in the previous categories. These programs and applications are as follows:

BOMJ  Using photon energies and uncertainties to develop level assignments.
COINC  To analyze coincident counting data.
CURVE  To determine the best fit to an arbitrary curve, useful, e.g., in determining Ge-detector efficiency curves.
DIMEN  To assist in assigning possible responsible nuclides for measured photon peaks.
GABAS  To generate time-dependent photon spectra from the output of an inventory-type program.
GASS  Compute self-shielding by an encapsulated photon source.
GRAP  Goal similar to that for BOMJ.
MARTHA  Compute NaI(Tl) scintillation-detector response functions.
MGA  Determines relative abundances of actinide isotopes from a spectrum obtained with a Ge-detector system.
PAPER.1  To compute solid angle and self-absorption factors for an inclined cylindrical source viewed by a cylindrical detector.
XRAY.AAC  To compute X-ray attenuation and absorption for any element.
1. NAME OR DESIGNATION OF PROGRAM - **BOMJ**.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
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<tr>
<td>BOMJ</td>
<td>IAEA246/01</td>
<td>IBM PC</td>
<td>IBM PC</td>
<td>AN</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

BOMJ uses measured gamma-ray energies with uncertainties and suggests level assignment to deduce a least-squares adjusted set of nuclear levels (similar to GTOL, see NESC-1149) and to find the places to dispose unassigned quanta among nuclear levels.

4. METHOD OF SOLUTION

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

204 nuclear levels, 1024 assigned quanta and 204 unassigned quanta.

6. TYPICAL RUNNING TIME

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS

A non-standard string handling routine F77STR; and conversion routines NSDCNV for NSD applications.

9. STATUS

IAEA1246/01 : Requested by NEADB
               : Arrived, no report

10. REFERENCES

- B.J. Barton, J.K. Tuli:
  "Physics Analysis Programs for Nuclear Structure Evaluation"
  BNL-NCS-23375/R, October 1977
IAEA1246/01 :
11. MACHINE REQUIREMENTS

A 350KB virtual drive is recommended. To run BOMJ.EXE, the virtual drive must be named E:
BOMJIC.EXE does not need a virtual drive, only hard disk space.

12. PROGRAMMING LANGUAGE USED

IAEA1246/01 : FORTRAN+ASSEMBLER

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

MS-DOS 4.1. The RM/FORTRAN compiler is required.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

F.E. Chukreev
C.A.J.A.D.
Kurchatov Institute
Moscow, Russia 123182

16. MATERIAL AVAILABLE

IAEA1246/01 :
ABSTRACT.TXT Abstract File
BOMJ.EXE Executable File
BOMJ.FOR Source File
BOMJ.LVL Test Case Data
BOMJIC.FOR Source File
README.DOC Information File
SHORT.RPT Short Report
TOTAL.RPT Total Report
PICTURE.LIB Symb. Data Lib.

17. CATEGORY = 0,

KEYWORDS ENSDF
data processing
evaluated data
gamma spectra
nuclear structure
1. NAME OR DESIGNATION OF PROGRAM. COINC.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
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<tr>
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<th>Test Computer</th>
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<td>COINC</td>
<td>NESC0248/02</td>
<td>CDC 3600</td>
<td>CDC 3600</td>
<td>T</td>
</tr>
</tbody>
</table>

3. NATURE OF PHYSICAL PROBLEM SOLVED.

Coincidence counting data are treated to obtain specific disintegration rates, channel efficiencies and count rates, weighted means, and all associated standard errors. Corrections are made for unequal deadtime loss in each channel, coincidence resolving time losses, decay during counting, decay from a reference time, and background in each of the three channels. Input variables include sample identification, start time for counting, sample reference time, counting interval, total number of counts in two single channels and one coincidence channel, and normalizing sample volume. Input parameters consist of deadtimes of each single channel, coincidence resolving time for all three channels, decay constant, background count rate for all three channels, and standard errors for each of the above parameters. Optional input allows date, group classification, and a 3-digit user code. Output contains corrected single channel, coincidence, and disintegration rates referred to start of count, specific disintegration rate (counts/second/unit volume or weight) referred to reference time, weighted mean and error of any number of problems in a group, efficiencies of the two independent detector channels, date, summary of background values used, identification number, count start time, and upper and lower limit (one standard deviation) of each of the computed quantities.

4. METHOD OF SOLUTION.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM.

   Decay constant greater than zero.
   500 problems per set for CDC3600.

6. TYPICAL RUNNING TIME.

10 seconds are required for a 50 card problem on the CDC3600.

7. UNUSUAL FEATURES OF THE PROGRAM.

A very simple input format is available, allowing application to essentially any coincidence decay scheme.
Input data may be transcribed by hand and punched from standard format onto cards, or automatically punched card data may be utilized. Modifications for paper tape are complete. Complex adjustments of the accidental coincidence rates affected by deadtime are made. Both Poisson statistics for total accumulated counts and error propagation for correlated and uncorrelated quantities are compounded in determination of standard deviations. The program was designed for absolute beta-gamma coincidence counting, but it has also been used for gamma-gamma and neutron-fission coincidence work. Compensation for radioactive decay can be made to any reference time for any number of days.

8. RELATED AND AUXILIARY PROGRAMS.

9. STATUS

NESC0248/01 : Arrived at NEADB
   : Tested at NEADB
   : Obsolete
NESC0248/02 : Arrived at NEADB
   : Tested at NEADB

10. REFERENCES.

NESC0248/01 :
NESC0248/02 :
- A. De Volpi, K.G. Porges and G. Jensen:
- G. Jensen:

11. MACHINE REQUIREMENTS.

12. PROGRAMMING LANGUAGE USED

NESC0248/01 : FORTRAN-II (IBM)
NESC0248/02 : FORTRAN-IV

13. OPERATING SYSTEM OR MONITOR UNDER WHICH PROGRAM IS EXECUTED. SCOPE

14. ANY OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS.

15. NAME AND ESTABLISHMENT OF AUTHOR.

   A. De Volpi, K. G. Porges, and G. Jensen
   Argonne National Laboratory
   9700 South Cass Avenue
   Argonne, Illinois 60439
16. MATERIAL AVAILABLE

NESC0248/01 :

Report:
SOURCE&DATA  0 records
OUTPUT       0 records

NESC0248/02 :
source program  mag tape
test-case data  mag tape
test-case output mag tape

Report: ANL 1198/RP-258 (June 9, 1966)
SOURCE %CDC 3600<  0 records
DATA            0 records
OUTPUT          0 records
SOURCE %CDC 3600<  0 records
DATA            0 records
OUTPUT          0 records

17. CATEGORY = O ,

KEYWORDS Statistics
data processing
decay
NEA CODE PACKAGE NESC9533

NESC9533 CURVE,LSFIT,GAMMA SPECTROMETER CALIBRATION BY INTERACTIVE FITTING
METH 900130

1. NAME OR DESIGNATION OF PROGRAM - CURVE,LSFIT.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>CURVE,LSFIT</td>
<td>NESC9533/01</td>
<td>DEC VAX 11/750</td>
<td>PC-80286</td>
<td>T</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

CURVE and LSFIT are interactive programs designed to obtain the best data fit to an arbitrary curve.

CURVE finds the type of fitting routine which produces the best curve. The types of fitting routines available are linear regression, exponential, logarithmic, power, least squares polynomial, and spline.

LSFIT produces a reliable calibration curve for gamma ray spectrometry by using the uncertainty value associated with each data point. LSFIT is intended for use where an entire efficiency curve is to be made starting at 30 KeV and continuing to 1836 KeV. It creates calibration curves using up to three least squares polynomial fits to produce the best curve for photon energies above 120 KeV and a spline function to combine these fitted points with a best fit for points below 120 KeV.

4. METHOD OF SOLUTION

The quality of fit is tested by comparing the measured y-value to the y-value calculated from the fitted curve. The fractional difference between these two values is printed for the evaluation of the quality of the fit.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Maxima of -
- 2000 data points calibration curve output (LSFIT)
- 30 input data points
- 3 least squares polynomial fits (LSFIT)

The least squares polynomial fit requires that the number of data points used exceed the degree of fit by at least two.

6. TYPICAL RUNNING TIME

7. UNUSUAL FEATURES OF THE PROGRAM

CURVE and LSFIT can operate in the executive mode, which is faster than BASIC and requires less memory.
8. RELATED AND AUXILIARY PROGRAMS

9. STATUS

NESC9533/01 : Requested by NEADB
   : Arrived "as is"
   : in preparation
   : Tested at NEADB

10. REFERENCES

NESC9533/01 :
- Dale G. Olson:
  Obtaining the Best Efficiency Curve by Curve Fitting Routines
- C. Yuleys-Miskis:
  CURVE,LSFIT Tape Description and Implementation Information
  NESC Note 88-101 (July 29, 1988).

11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

NESC9533/01 : BASIC

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

VMS 4.6.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

Compilation must be done with the GFloat qualifier.

15. NAME AND ESTABLISHMENT OF AUTHORS

D.G. Olson
Radiological & Environmental Sciences Laboratory
 Idaho Operations Office

16. MATERIAL AVAILABLE

NESC9533/01 :
CURVE BASIC Source, curve fitting program
LSFIT BASIC Source, gamma-ray spectrometry
How to use by D.G. Olson
NESC Note 88-101 (July 29, 1988)
Information file 114 records
CURVE.BAS CURVE source (Turbo Basic) 627 records
CURVEVAX.BAS CURVE source (VAX Basic) 614 records

118
<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
<th>Records</th>
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</thead>
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<tr>
<td>LSFIT.BAS</td>
<td>LSFIT source (Turbo Basic)</td>
<td>536</td>
</tr>
<tr>
<td>LSFITVAX.BAS</td>
<td>LSFIT source (VAX Basic)</td>
<td>522</td>
</tr>
<tr>
<td>CURVE.EXE</td>
<td>CURVE executable file</td>
<td>0</td>
</tr>
<tr>
<td>LSFIT.EXE</td>
<td>LSFIT executable file</td>
<td>0</td>
</tr>
<tr>
<td>XDATA.FIT</td>
<td>Sample input</td>
<td>29</td>
</tr>
<tr>
<td>YDATA.FIT</td>
<td>Sample input</td>
<td>29</td>
</tr>
<tr>
<td>ZDATA.FIT</td>
<td>Sample input</td>
<td>29</td>
</tr>
<tr>
<td>CURVE.OUT</td>
<td>CURVE sample output</td>
<td>75</td>
</tr>
<tr>
<td>LSFIT.OUT</td>
<td>LSFIT sample output</td>
<td>133</td>
</tr>
<tr>
<td>DOS</td>
<td>file-names</td>
<td>12</td>
</tr>
</tbody>
</table>

17. CATEGORY = 0,

KEYWORDS gamma spectra
least square fit
spectra unfolding
spectrometers
spline functions
1. NAME AND TITLE
   **DIMEN:** Code System for Isotope Identification by Gamma-Ray Analysis.

2. CONTRIBUTOR
   Riga Radioisotope Research Institute, Riga, Latvia.

3. CODING LANGUAGE AND COMPUTER
   Pascal; IBM PC (P00341/IBMPC/00).

4. NATURE OF PROBLEM SOLVED
   For a set of a priori given nuclides taken from a work library, DIMEN uses median estimates of the peak areas and estimates of their errors to produce a list of possible nuclides matching a gamma-ray line and some measure of the reliability of this assignment.

5. METHOD OF SOLUTION
   The identification of a given radionuclide is obtained by searching for a match with the energy information of a database. This procedure is performed in an interactive graphic mode by markers that superimpose, on the experimental data, the energy information provided by a previously elaborated data library. This library of experimental data includes approximately 16682 gamma-energy lines related to 749 known gamma emitter radioisotopes currently listed by the ICRP.

6. RESTRICTIONS OR LIMITATIONS
   Number of channels: 4096.

7. TYPICAL RUNNING TIME
   Interactive. No timing was attempted.

8. COMPUTER HARDWARE REQUIREMENTS
   The code was tested on a PC 486 but should run on all IBM PC compatible computers.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code was written in Pascal. The original source code file was broken into several units by RSIC to test compilation using Microsoft QuickPascal.

10. REFERENCES
    Informal Notes: "Description of the MAKEBASE and DIMEN Programs" (1995).

11. CONTENTS OF CODE PACKAGE
    Included are the referenced documents and 2 3.5-in. DS/DD (1.44 MB) diskettes written in DOS format.
DATE OF ABSTRACT
January 1996.

KEYWORDS: GAMMA-RAY SPECTRUM ANALYSIS; RADIONUCLIDES; INTERACTIVE, ON-LINE; MICROCOMPUTER
RSICC CODE PACKAGE PSR-175

1. NAME AND TITLE

   AUXILIARY ROUTINES
   ISPEC: Reads fission product spectral data and writes a binary file for input to GABAS.

2. CONTRIBUTORS
   Instrumentation Research Technology, San Diego, California.
   Sandia National Laboratories, Albuquerque, New Mexico.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; UNIVAC 1100/81.

4. NATURE OF PROBLEM SOLVED
   GABAS calculates time-dependent beta- and/or gamma-ray spectra from decaying fission products.

5. METHOD OF SOLUTION
   GABAS calculates composite fission-product beta and/or gamma-ray spectra based on the technique
   used by England, et al., in conjunction with the CINDER family of fission product codes. Multigroup
   beta and gamma-ray spectra for individual nuclides are folded with their corresponding time-dependent
   activities (usually generated by a fission product inventory code) to produce a composite time-dependent
   fission product spectrum. GABAS was intended to interface with the fission product inventory code
   RIBD-IRT; however, other codes like ORIGEN or CINDER could be utilized with appropriate
   modifications to their output format.

6. RESTRICTIONS OR LIMITATIONS
   None noted.

7. TYPICAL RUNNING TIME
   For 34 time steps and 180 fission products, the approximate CPU time was 10 seconds.

8. COMPUTER HARDWARE REQUIREMENTS
   GABAS is operable on the UNIVAC 1100/81 computer. Two mass storage files, either tapes or
   discs, and a printer are needed.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.

10. REFERENCES
    a. Included in documentation:

    b. Background information:

11. CONTENTS OF CODE PACKAGE
Included are the referenced document (a) and a reel of magnetic tape which contains the source program and sample problem input written in EBCDIC card images; total records 2565.

12. DATE OF ABSTRACT
February 1982; August 1984.

KEYWORDS: DATA PROCESSING, SPECTRA; GAMMA-RAY SPECTRUM ANALYSIS; RADIATION SOURCE GENERATOR
1. NAME AND TITLE
   **GASS:** Monte Carlo Calculation of Self Shielding by Encapsulated Gamma-Ray Sources.

   This code package originated in Office of Civil Defense programs in 1966; is retained by RSIC to preserve the technology.

2. CONTRIBUTORS
   University of Illinois, Civil Engineering and Nuclear Engineering Program, Urbana, Illinois.

3. CODING LANGUAGE AND COMPUTER
   FORTRAN IV; IBM 7090 and 7094.

4. NATURE OF PROBLEM SOLVED
   GASS was designed to calculate the energy and angular distributions of photons emitted from a cylindrical or spherical encapsulated source.

5. METHOD OF SOLUTION
   GASS represents an approximate solution by Monte Carlo methods to the steady state transport equation.

   A time-saving procedure utilizing a "do-nothing" cross section allows ray tracing to proceed without many cross section look-ups and partial path length calculations. A choice is then made where the collision occurs between scattering, absorption, or the straight-ahead "do-nothing" reaction.

6. RESTRICTIONS OR LIMITATIONS
   There are no known restrictions implied by storage allocation.

7. TYPICAL RUNNING TIME
   Processing of 20,000 histories in the sample problem required 3 minutes on the IBM 7090 and 1.3 minutes on the 7094.

8. COMPUTER HARDWARE REQUIREMENTS
   The code was designed for the 32 K IBM 7094 computer with 3 tape units.

9. COMPUTER SOFTWARE REQUIREMENTS
   The code may be compiled and executed on the IBM FORTRAN IV IBJOB Monitor and other compatible systems. Standard I-O and systems tape assignments are made.

10. REFERENCE

11. CONTENTS OF CODE PACKAGE
    Included are the referenced document and a reel of magnetic tape which contains the source code and input for a sample problem written in BCD/EBCDIC card images and an output listing from running the problem; total records 734.
12. DATE OF ABSTRACT

KEYWORDS: MONTE CARLO; GAMMA-RAY; RAY-TRACING
1. NAME OR DESIGNATION OF PROGRAM - GRAP.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

Program-name Package-ID Orig. Computer Test Computer Status
----------------- ----------- ---- ----------- ---
GRAP IAEA1175/01 IBM PC IBM PC A

3. DESCRIPTION OF PROGRAM OR FUNCTION

An interactive program for allocating gamma-rays to an energy level scheme. Procedure allows for searching for new candidate levels of the form:
1) L1 + G(A) + G(B) = L2
2) G(A) + G(B) = G(C)
3) G(A) + G(B) = C (C is a user defined number)
4) L1 + G(A) + G(B) + G(C) = L2

Procedure indicates intensity balance of feed and decay of each energy level. Provides for optimization of a level energy (and associated error). Overall procedure allows for pre-defining of certain gamma-rays as belonging to particular regions of the level scheme, for example, high energy transition levels, or due to beta-decay.

4. METHOD OF SOLUTION

Search for cases in which the energy difference between two energy levels is equal to a gamma-ray energy within user-defined limits.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

<table>
<thead>
<tr>
<th>Maximum number of gamma-rays</th>
<th>999</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum gamma ray energy</td>
<td>32000 units</td>
</tr>
<tr>
<td>Minimum gamma ray energy</td>
<td>10 units</td>
</tr>
<tr>
<td>Maximum gamma-ray intensity</td>
<td>32000 units</td>
</tr>
<tr>
<td>Minimum gamma-ray intensity</td>
<td>0.001 units</td>
</tr>
<tr>
<td>Maximum number of levels</td>
<td>255</td>
</tr>
<tr>
<td>Maximum level energy</td>
<td>32000 units</td>
</tr>
<tr>
<td>Minimum level energy</td>
<td>10 units</td>
</tr>
<tr>
<td>Maximum error on energy, intensity</td>
<td>32 units</td>
</tr>
<tr>
<td>Minimum error on energy, intensity</td>
<td>0.001 units</td>
</tr>
<tr>
<td>Maximum number of combinations</td>
<td>6400 (ca)</td>
</tr>
<tr>
<td>Maximum number of gamma-ray types</td>
<td>127</td>
</tr>
</tbody>
</table>

6. TYPICAL RUNNING TIME

127
Highly dependent on the number of transitions to be allocated and errors used. To generate the initial scheme (CRAG1) takes typically 10-15 minutes for 800 gamma-rays fitting to 120 levels.

7. UNUSUAL FEATURES OF THE PROGRAM

Intensity balance display of the feeding level and decaying level for particular transition gamma-ray energies.

Selective inclusion/removal of gamma-rays in multiple fit situation. Ability to force fit of gamma-ray even though errors dictate outside acceptance window.

8. RELATED AND AUXILIARY PROGRAMS

TRED - Raw data input, and edit, program.
GRAG1 - Preliminary assignment program.

9. STATUS

IAEA1175/01 : Requested by NEADB
: Arrived at NEADB

10. REFERENCES

- C. Hofmeyr et al:
  74GE: Transitions and Levels Excited in Thermal-Neutron Capture
  AIP Conference Proceedings No. 125 - Capture Gamma-Ray
  Edited by S. Raman, pages 378-381.

IAEA1175/01 :
- C.B. Franklyn:
  GRAP - Gamma Ray Allocations Program - A User's Guide
  PEL-286 (May 1985)

11. MACHINE REQUIREMENTS

HP-version: HP-1000 series minicomputer, 192 Kbytes memory, disc drive, magnetic tape, terminal/monitor.
PC-version: IBM-PC XT or compatible, 512 Kbytes RAM, disc drive, printer, maths coprocessor (optional).

12. PROGRAMMING LANGUAGE USED

IAEA1175/01 : FORTRAN

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

HP version: Designed on RTE-IV B system, runs on RTE-VI.
PC version: MS-DOS 3.2 or higher.
14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

HP version: makes system calls to LOGLU, EXEC, OPEN, READF, WRITF, CLOSE, RMPAR, LURQ, IFBRK, FTIME. The printer for which the program was originally designed was a HP7310A.

15. NAME AND ESTABLISHMENT OF AUTHORS

Dr. C.B. Franklyn
Nuclear Energy Systems
Atomic Energy Corporation of South Africa
P.O. Box 582, Pretoria, South Africa

16. MATERIAL AVAILABLE

README File
GRAP Source Programs (HP Computer) (FTN4)
GRAG1 Source Programs (HP Computer) (FTN4)
TRED Source Programs (HP Computer) (FTN4)
GRAPEM Data File (HP Computer)
TREDED Data File (HP Computer)
1TRED Source Program (IBM PC/XT)
1CRAG1 Source Program (IBM PC/XT)
1GRAP Source Program (IBM PC/XT)
TREDED Data File (IBM PC/XT)
GRAPEM Data File (IBM PC/XT)
TREDTEST/CRAGTEST/GRAPTEST Data Files
README.TXT from DISC 1 & 2
Source Programs (4 files)
Data for TRED
Sample Output from GRAP
Sample Output from GRAG

17. CATEGORY = 0,

KEYWORDS gamma spectra
multilevel analysis
spectra unfolding
NEA CODE PACKAGE NEA 0983

NEA 0983 MARTHA, NAI(Tl) GAMMA SCINTILLATION DETECTOR_RESPONSE BY M-C 860314

1. NAME OR DESIGNATION OF PROGRAM - MARTHA.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>MARTHA</td>
<td>NEA 0983/01</td>
<td>FACOM M-380</td>
<td>IBM 3084Q</td>
<td>T</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

The program MARTHA calculates NaI(Tl) scintillation detector response functions to gamma rays. There are four versions of the program according to the detector shape and gamma-ray energy.

4. METHOD OF SOLUTION

Using a Monte Carlo method, every photon and electron produced by one incident photon are traced in a detector assembly, and the total energy deposited in the crystal is recorded as a pulse height. Repeating this procedure several times, a response function is obtained.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

Response functions can be calculated for cylindrical or spherical detectors. The program was originally designed to calculate response functions for gamma energies from 0.01 MeV to 10 MeV. But the program should work up to 20 MeV. Available source conditions are a point source on the detector axis and a parallel beam. The maximum channel number of a spectrum is 300.

6. TYPICAL RUNNING TIME

Running time depends among other factors on the incident gamma energy. For 10,000 gamma quants of 1.0 MeV incident on a 3 in. x 3 in. cylindrical crystal, execution time is approximately 11 seconds on an FACOM 380.

NEA 0983/01: NEA-DB executed the test cases included in this package on an IBM 3084Q computer. The following CPU times were required: 22 seconds (version 1); 15 seconds (version 2); 53 seconds (version 3); 21 seconds (version 4).

7. UNUSUAL FEATURES OF THE PROGRAM

The program takes the following two effects into account: (1) The housing material of the NaI(Tl) crystal; (2) the non-linear response of a NaI(Tl) detector to electron energy.

8. RELATED AND AUXILIARY PROGRAMS
Five programs to prepare the input data for MARTHA. These data are already given in the sample input.

9. STATUS

NEA 0983/01: Arrived at NEADB

: in preparation

: Tested at NEADB

10. REFERENCES

- K. Saito and S. Moriuchi:
  Monte Carlo Calculation of Accurate Response Functions for a NaI(Tl) Detector for Gamma Rays.
  Reprinted from: Nuclear Instruments & Methods, 185(1981)299-308
- K. Saito and S. Moriuchi:
  Monte Carlo Calculation of Accurate Response Functions for a NaI(Tl) Detector for Gamma Rays and
  Analysis of Pulse Height Spectrum Formation Mechanism.
  JAERI-M 9741 (In Japanese) (September 1981)

11. MACHINE REQUIREMENTS

NEA 0983/01: The test cases were run in 550K bytes of IBM 3084Q main storage.

12. PROGRAMMING LANGUAGE USED

NEA 0983/01: FORTRAN-IV

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

FACOM OS 4-F4-MSP.

NEA 0983/01: MVS-SP (IBM 3084Q).

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

K. Saito
Department of Environmental Safety Research
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken
Japan

16. MATERIAL AVAILABLE

Source Program (Fortran-IV) (Version 1)
Subroutine Source (Fortran-IV) (Version 1)
Sample Input (Version 1)
Input Library (FT31) (Version 1)
Input Library (FT32) (Version 1)
Input Library (FT33) (Version 1)
JCL (Version 1)
Sample Output (Version 1)
Source Program (Fortran-IV) (Version 2)
Subroutine Source (fortran-IV) (Version 2)
Sample Input (Version 2)
JCL (Version 2)
Sample Output (Version 2)
Source Program (Fortran-IV) (Version 3)
Subroutine Source (fortran-IV) (Version 3)
Sample Input (Version 3)
Input Library (FT33) (Version 3)
Input Library (FT32) (Version 3)
Input Library (FT33) (Version 3)
JCL (Version 3)

NEA 0983/01:
Sample Output (Version 3)
Source Program (Fortran-IV) (Version 4)
Subroutine Source (fortran-IV) (Version 4)
Sample Input (Version 4)
JCL (Version 4)
Sample Output (Version 4)


Input Description
This information file 119 records
Program to convert EBCDIC to binary 26 records
Routine RANDOM from SLATEC library 117 records
Program MARTHA source. Version 1 2496 records
JCL to run MARTHA version 1 101 records
Input for version 1 57 records
Library for version 1 (file code 31) 216 records
Library for version 1 (file code 32) 594 records
Library for version 1 (file code 33) 540 records
Test case output, version 1 768 records
Program MARTHA source, version 2 1972 records
JCL to run version 2 74 records
Input for version 2 20 records
Test case output,version 2 425 records
Program MARTHA source, version 3 1968 records
JCL to run version 3 101 records
Input for version 3 48 records
Library for version 3 (file code 31) 216 records
Library for version 3 (file code 32) 594 records
Library for version 3 (file code 33) 540 records

133
Test case output, version 3 1076 records
Program MARTHA source, version 4 1557 records
JCL to run version 4 74 records
Input for version 4 15 records
Test case output, version 4 663 records

17. CATEGORY = 0,

KEYWORDS gamma detectors
response functions
scintillation detectors
NEA CODE PACKAGE NESC9479

NESC9479 MGA, PU ISOTOPE ABUNDANCE FROM MULTICHANNEL ANALYZER GAMMA SPECTRA
930309

1. NAME OR DESIGNATION OF PROGRAM - MGA.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED

<table>
<thead>
<tr>
<th>Program-name</th>
<th>Package-ID</th>
<th>Orig. Computer</th>
<th>Test Computer</th>
<th>Status</th>
</tr>
</thead>
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<tr>
<td>MGA</td>
<td>NESC9479/01</td>
<td>DEC VAX series</td>
<td>DEC VAX 8810</td>
<td>T</td>
</tr>
<tr>
<td>MGA</td>
<td>NESC9479/02</td>
<td>IBM PC</td>
<td>IBM PC</td>
<td>K</td>
</tr>
</tbody>
</table>

3. DESCRIPTION OF PROGRAM OR FUNCTION

The MGA (Multiple Group Analysis) program determines the relative abundances of plutonium and other actinide isotopes in different materials. The program analyzes spectra taken of such samples using a 4096-channel germanium (Ge) gamma-ray spectrometer. The code can be run in a one or two detector mode. The first spectrum which is required and must be taken at a gain of .075 Kev/channel with a high resolution planar detector, contains the 0-300Kev energy region. The second spectrum, which is optional, must be taken at a gain of 0.25 Kev/channel; it becomes important when analyzing high burnup samples (concentration of Pu(241) greater than one percent). Isotopic analysis precisions of one percent or better can be obtained, and no calibrations are required. The system also measures the abundances of U(235,238), Np237, and Am241. A special calibration option is available to perform a one-time peak-shape characterization when first using a new detector system.

4. METHOD OF SOLUTION

The basic method for determining the relative abundance of the isotopes of plutonium is to measure the intensity of two or more peaks from gamma rays of similar energy, but arising from different isotopes. Since the gamma-ray emission probabilities and half-lives are known, the atom ratios can be calculated provided relative detection efficiencies for the peaks can be estimated.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM

6. TYPICAL RUNNING TIME

Analysis time is less than one minute.

7. UNUSUAL FEATURES OF THE PROGRAM

8. RELATED AND AUXILIARY PROGRAMS
9. STATUS

NESC9479/01: Offered to NEADB
  : Requested by NEADB
  : Arrived "as is"
  : in preparation
  : Tested at NEADB

NESC9479/02: Requested by NEADB
  : Known to NEADB

10. REFERENCES

- R. Gunnink:
  MGA2 - A One-Detector Code for Rapid High-Precision Plutonium Measurements
  UCRL-96016 Rev. 1, Preprint (July 1987).
NESC9479/01:
- R. Gunnink:
  MGA - A Gamma-Ray Spectrum Analysis Code for Determining Plutonium Isotopic Abundances Volume
- R. Gunnink:
  A New One-Detector Analysis Method for Rapid High-Precision Plutonium Isotopic Measurements
  Reprinted from the Proceedings of the 9th ESARDA Symposium on Safeguards and Nuclear Material

11. MACHINE REQUIREMENTS

12. PROGRAMMING LANGUAGE USED

NESC9479/01: FORTRAN-77
NESC9479/02: FORTRAN-77

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED

VMS.
NESC9479/01: The program was compiled by NEA-DB on a DEC VAX 8810 computer under VMS
V5.4-2 using the DEC/VAX FORTRAN-77 compiler. The test case was run interactively.

14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

15. NAME AND ESTABLISHMENT OF AUTHORS

R. Gunnink
Lawrence Livermore National Laboratory

16. MATERIAL AVAILABLE

NESC9479/01:
MGA Source File
Executable Image
Object Modules
Object Library
Sample Problem Data (BINARY)
Auxiliary Information
Control Information
Sample Output
ESARDA Reprint
Information file 102 records
000004.Z17 0 records
000575.H27 0 records
AVE FOR 0 records
BKG.D.FOR 103 records
BKG.RD.FOR 131 records
BWF.FOR 71 records
C2JDAT.FOR 24 records
CALERR.FOR 20 records
FOR007.DAT Sample problem output 103 records

NESC9479:
GFIT.FOR 102 records
GRP100.DAT 31 records
GRP340.DAT 22 records
GRP660.DAT 18 records
J2CDAT.FOR 30 records
MATINV.FOR 80 records
MAXVAL.FOR 48 records
MGA.COM 16 records
MGA.FOR 129 records
MGA.RUN 5 records
MGA100.FOR 353 records
MGA235.FOR 174 records
MGA300.CMN 31 records
MGA300.FOR 253 records
MGA45.FOR 178 records
MGA600.FOR 250 records
MGA94.FOR 636 records
MGAABS.FOR 548 records
MGACAL.CMN 5 records
MGACAL.FOR 545 records
MGACOM.CMN 104 records
MGADAT.CMN 8 records
MGAEQS.FOR 273 records
MGAGAN.FOR 250 records
MGAHIE.FOR 528 records

137
MGAOUT.FOR 307 records
MGAPKS.FOR 437 records
MGASPC.FOR 461 records
NCNTS.FOR 61 records
PKFIT.CMN 4 records
PKFIT.FOR 691 records
RDCHN.FOR 9 records
RDCHN2.FOR 54 records
RDCHN3.FOR 58 records
SHAPC.Z1 15 records
SHAPC2.H2 10 records
SPRAM.FOR 85 records
STRIP1.FOR 85 records
UTFSBS.FOR 397 records
UTLIB.OLB 0 records

17. CATEGORY = D, O,

KEYWORDS plutonium spectra
RSICC COMPUTER CODE PSR-097

1. NAME AND TITLE
   PAPER 1: Monte Carlo Calculation of Solid Angle and Self-Absorption Factors for an Inclined Cylindrical Source Viewed by a Cylindrical Detector.

2. CONTRIBUTOR
   Department of Physics, Ben Gurion University of the Negev, Beersheva, Israel.

3. CODING LANGUAGE AND COMPUTER
   Fortran IV; CDC 6600.

4. NATURE OF PROBLEM SOLVED
   PAPER 1 calculates the self absorption of gamma radiation in an inclined cylindrical source and, also, the solid angle of the source subtended by a cylindrical detector. It can be used in any situation in which a transformation composed of a translation and a rotation between the source and detector coordinate systems is required.

5. METHOD OF SOLUTION
   PAPER 1 uses the Monte Carlo method for determining self-absorption and solid-angle correction factors in the inclined cylindrical geometry. The Monte Carlo method used in PAPER 1 is extremely flexible and many geometric configurations can be treated with only trivial modifications of the computer program.

6. RESTRICTIONS OR LIMITATIONS
   No weighting factor was assigned to the gamma ray as a function of its angle of incidence on the detector.

7. TYPICAL RUNNING TIME
   The Monte Carlo method for determining self-absorption and solid-angle correction factors in the inclined cylindrical geometry requires fairly large amounts of computer time to acquire statistical accuracy of the order of 1%. A total of 1000 s of computer time was used to run 40,000 case histories per point on the CDC-6000 computer.

8. COMPUTER HARDWARE REQUIREMENTS
   PAPER 1 is operable on the CDC 6600 computer.

9. COMPUTER SOFTWARE REQUIREMENTS
   A Fortran IV compiler is required.

10. REFERENCES
    "User's Instructions," Informal Note.
11. CONTENTS OF CODE PACKAGE
    Included are the referenced documents and a reel of magnetic tape which contains the source code input written in EBCDIC card images; total records 76.

12. DATE OF ABSTRACT
    March 1984.

    KEYWORDS: GAMMA-RAY SOURCE ANALYSIS; SELF ABSORPTION
RSICC CODE PACKAGE CCC-525

1. NAME AND TITLE
   XRAY_AAC: X-ray Attenuation and Absorption Calculations.

AUXILIARY ROUTINES
   UPDATE_COEFF: Convert data library to binary indexed file.
   AAC_1: Application program to demonstrate calling XRAY_AAC.
   AAC_2: Interactive application program to call XRAY_AAC.
   AAC_3: Interactive application program to provide easy access to Function XRAY_AAC.

DATA LIBRARY
   ELEMENTS.DAT: Subset of DLC-99/HUGO including attenuation and absorption coefficients.

2. CONTRIBUTOR

3. CODING LANGUAGE AND COMPUTER
   Fortran 77; VAX.

4. NATURE OF PROBLEM SOLVED
   This point-source, polychromatic, discrete energy X-ray transport and energy deposition code system
calculates first-order spectral estimates of X-ray energy transmission through slab materials and the
associated spectrum of energy absorbed by the material.

5. METHOD OF SOLUTION
   X-ray source spectra may be internally generated and normalized (Kramer or Planck spectrum), read
from data files, or read from an electronic library. Virtually any material consisting of the first 100
atomic elements may be specified as a shield or absorber using a common symbolic format. The
calculated spectra may be selectively written to data files which in turn may be used as input to further
calculations. One aspect of this software that is believed unique is its ability to parse chemical
compounds and alloys that are entered in a conventional symbolic format and calculate the relative mass
of the constituent elements.

6. RESTRICTIONS OR LIMITATIONS
   Because this software is written in Vax Fortran, which is a superset of ANSI Fortran 77, and takes
appropriate advantage of VMS system routines and run-time library functions, its transportability is
limited.

7. TYPICAL RUNNING TIME
   The programs take only a few seconds to execute interactively.

8. COMPUTER HARDWARE REQUIREMENTS
   The codes run on VAX 11/750 or VAX 8600 computers.
9. COMPUTER SOFTWARE REQUIREMENTS  
The codes were developed using Vax/VMS Version 4.5 and Vax Fortran Version 4.6.

10. REFERENCE  

11. CONTENTS OF CODE PACKAGE  
Included are the referenced document and one DS/HD 5.25 (1.2MB) diskette in compressed DOS files.

12. DATE OF ABSTRACT  

KEYWORDS: BEAM TRANSPORT; ENERGY DEPOSITION; GAMMA-RAY SOURCE; GAMMA-RAY; INTERACTIVE; X-RAY
SECTION 6
DATA LIBRARIES

These libraries contain photon energies and branching ratios of decay gamma rays. These data are used in identification of isotopes responsible for data observed in measured photon spectra.

As in the case of computer codes discussed in previous sections, these compilations reflect scientific evaluations usually related to an ongoing experimental program (or programs), and may be written for specific computer environments. Although there is a substantial overlap in the information presented, the individual data libraries are unique. The compilers do not make a recommendation for the choice of library to use.
1. NAME AND TITLE OF DATA LIBRARY
   GAMDAT-78: Library of Gamma-Ray Decay Data for 2055 Radionuclides.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS
   No retrieval program is included in the package.

3. CONTRIBUTOR
   Central Division of Chemical Analysis, Nuclear Research Establishment, Jülich, Federal Republic of Germany.

4. HISTORICAL BACKGROUND AND INFORMATION
   Gamma-ray spectrometry, which in every case includes the step of gamma-ray spectra evaluation, is an indispensable tool in nearly all fields where radioactive materials and substances are handled or investigated.

5. APPLICATION OF THE DATA
   However, not only in connection with the production of energy by nuclear fission is gamma-ray spectrometry required. Fusion reactors also will produce radioactive materials and must use this method. Gamma-ray spectrometry is also vital to nuclear medicine and gamma-ray spectrometry is the most important measuring technique used in radioanalytical chemistry, as well as planning for the shielding required for radioactive materials.

6. SOURCE AND SCOPE OF DATA
   Starting from a collection of gamma-ray data used for gamma-ray spectra evaluation in the authors' laboratory, this data set was completed by systematic compilation of all gamma-ray data available. The first edition of the data collections was available in 1973; in 1978 an updated, completed and corrected version was finished.
   The latest version contains 1) all radionuclides known until 1977; 2) their half-lives; 3) their daughter-nuclides; 4) their long-lived precursor-nuclides (parents); 5) their genesis or mode of artificial production; 6) hints to the references where the gamma-ray data have been found; 7) the energies of the gamma-ray and X-ray lines; 8) the abundances (intensities) of the gamma rays and X-rays.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM
   Not applicable.

8. DATA FORMAT AND COMPUTER
   EBCDIC card images; IBM 370/3033.

9. TYPICAL RUNNING TIME
   Not applicable.

10. REFERENCE
11. CONTENTS OF LIBRARY
   Included are the referenced document and a reel of magnetic tape which contains the radionuclide
gamma-ray data file GAMDAT 78; total records 52,015.

12. DATE OF ABSTRACT
   April 1985.

   KEYWORDS: RADIOACTIVE DECAY SPECTRA
RSICC DATA LIBRARY DLC-032

1. NAME AND TITLE OF DATA LIBRARY
   GAMTAB: Radioactive-Decay Gamma-Rays Ordered by Energy and Nuclide.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAM
   No retrieval program is included in the package.

3. CONTRIBUTOR
   Savannah River Laboratory, Aiken, South Carolina, through the Argonne Code Center, Argonne, Illinois.

4. HISTORICAL BACKGROUND AND INFORMATION
   Since the first Catalogue of Gamma-Rays Emitted by Radionuclides was published by M. A. Wakat in 1971, the continued use of Ge(Li) detectors of high resolution has resulted in a general upgrading of nuclear decay data. The present work consists of data from the original catalogue card files with additions and corrections where newer, superior data were at hand.

5. APPLICATION OF THE DATA
   Because of the increased precision of the revised data, several minor policy changes were made to allow for: 1) Energy listings to 0.01 keV, where available; 2) Uncertainty listings for the energy, where available; 3) Use of exponential notation for half-lives and gamma-ray abundances; 4) Revision of the production mode code; 5) Listing the two most-abundant associated gamma rays to the nearest keV.

6. SOURCE AND SCOPE OF DATA
   GAMTAB has a separate table of the data listed by nuclide. By means of the original Catalogue, the source of a gamma ray could be narrowed initially via two associated gamma rays to several possibilities. However, to reduce these possibilities to one, much further searching through the Catalogue and spectrum was required. In this work, TABLE II, the listing by nuclide of up to 50 associated gammas, will allow a more rapid and thorough search of the data for each of the possible nuclides and eliminate the less abundant gamma rays from further scrutiny.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM
   Not applicable.

8. DATA FORMAT AND COMPUTER
   EBCDIC card images; IBM 360/370.

9. TYPICAL RUNNING TIME
   No study has been made by RSICC of typical running times for GAMTAB.

10. REFERENCE

11. CONTENTS OF LIBRARY
    Included are the referenced document and a reel of magnetic tape which contains the gamma-ray data
listed in ascending energy, data listed by nuclide, and references written in EBCDIC card images; total records 26,871.

12. DATE OF ABSTRACT
June 1984.

KEYWORD: RADIOACTIVE DECAY SPECTRA
1. NAME AND TITLE OF DATA LIBRARY
   GAMTOT78: Compilation of Radioactive Decay and Capture Gamma Rays.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAM
   GAMIDEN: An Aid to the Identification of Unknown Materials through Gamma-Ray Spectroscopy.

3. CONTRIBUTOR
   Lawrence Livermore Laboratory, Livermore, California.

4. HISTORICAL BACKGROUND AND INFORMATION
   The intent of GAMIDEN is to help identify isotopes by their gamma-ray emissions and, thus, to assist in the nondestructive assay of unknown materials from both radioactive decay and neutron captures.

5. APPLICATION OF THE DATA
   GAMIDEN searches GAMTOT78, a file of gamma-ray spectra, for matches with observed photon energies. The gamma-rays emitted by an isotope undergoing radioactive decay or neutron capture have energies and intensities that are characteristic of that isotope. A useful method for the nondestructive assay of unknown materials is based on identifying the signature of the isotope.
   Since there are thousands of known gamma-rays, the automated search procedure searches for isotopes that satisfy the input criteria. Each such isotope is printed out, accompanied by a list of other gamma emissions from the isotope that one might expect to see.
   The data file is taken from two compilations of gamma-ray spectra. The compilation of radioactive-decay gammas includes the half-life for each isotope and the energy and probability of emission per decay for each gamma emitted by that isotope.

6. SOURCE AND SCOPE OF DATA
   Included are photon energies greater than 1 MeV and probabilities greater than 0.01. A total of 43,940 entries are provided.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM
   GAMIDEN lists the matching isotopes, eliminates isotopes that are likely to be the source of the observed protons, and then lists the isotopes that are left. It is designed for the Cray 1. It is written in standard Fortran (ANSI), but contains some LRLTRAN instructions to make use of the Livermore time-sharing system.

8. DATA FORMAT AND COMPUTER
   Character type EBCDIC; GAMTOT78 data 120 character records, Cray 1, IBM 3033.

9. TYPICAL RUNNING TIME
   For GAMIDEN, the typical problem requires less than 0.75 min. Please note that disk file GAMTOT78 must be present. No input data required.
10. REFERENCES
   a. Included in the documentation:

   b. Background information:

11. CONTENTS OF LIBRARY
   Included are the referenced document (a) and a reel of magnetic tape which contains the program to search the data file and the data file written in BCD/EBCDIC card images; total records 44,390.

12. DATE OF ABSTRACT
   March 1984.

   KEYWORD: RADIOACTIVE DECAY SPECTRA
1. NAME AND TITLE OF DATA LIBRARY

NFCLIST: Radionuclide Radiation Data from the Evaluated Nuclear Data File (ENDF/B) for Routine Releases from Nuclear Fuel Cycle Facilities.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS

No retrieval program is in the package.

3. CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

4. HISTORICAL BACKGROUND AND INFORMATION

The calculation of radiation doses from exposure to radionuclides requires a knowledge of the energies and intensities of the atomic and nuclear radiations emitted during the decay process. NFCLIST provides tabulations of decay data for radionuclides expected to occur in routine releases of effluents from nuclear fuel cycle facilities.

5. APPLICATION OF THE DATA

NFCLIST gives tabulations of the atomic and nuclear radiations emitted by 240 radionuclides. Most of these are the ones expected to occur in routine releases of effluents from nuclear fuel cycle facilities. The half-life and recommended values for the energies, intensities, and equilibrium absorbed-dose constants for each of the atomic and nuclear radiations are given for each radionuclide. Also given are the daughter radionuclides produced and recommended values for decay branching ratios, where applicable. The radioactivity decay chains and branching ratios are displayed in diagram form.

6. SOURCE AND SCOPE OF DATA

Most of the decay data are for the radionuclides given in Table A-3 of Regulatory Guide 1.109, USNRC, and their radioactive daughter products.

Nuclear fuel cycle data was contributed by ORNL Nuclear Data Project. The data are taken from atomic and nuclear radiations emitted by 240 radionuclides which are expected to occur in routine releases of effluents for nuclear fuel cycle facilities. They were derived from a computer file used to prepare NUCLEAR DATA SHEETS (the Evaluated Nuclear Structure Data File).

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM

Not applicable.

8. DATA FORMAT AND COMPUTER

EBCDIC card images; IBM 360.

9. TYPICAL RUNNING TIME

Not applicable.

10. REFERENCE

11. CONTENTS OF LIBRARY
   Included are the referenced document and a reel of magnetic tape which contains the decay data and the MEDPRINT source file written in EBCDIC card images, plus output from the sample problem; total records 38,175.

12. DATE OF ABSTRACT
   March 1985.

   KEYWORDS:  RADIOACTIVE DECAY SPECTRA
RSICC DATA LIBRARY DLC-172

1. NAME AND TITLE OF DATA LIBRARY
   NUCDECAY: Nuclear Decay Data for Radiation Dosimetry Calculations for ICRP and MIRD.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS
   DEXRAX: Extracts decay data from the library for radionuclide(s) specified by the user.

3. CONTRIBUTOR
   Oak Ridge National Laboratory, Oak Ridge, Tennessee.

4. HISTORICAL BACKGROUND AND INFORMATION
   The Dosimetry Research Group (DRG) of the Health Sciences Research Division at ORNL has for several years maintained data bases of nuclear decay data for use in dosimetric calculations. The data on mean and unique energy plus intensity have been previously published, in abridged form, in Publication 38 of the International Commission on Radiological Protection (ICRP 1983) and a monograph for the Medical Internal Radiation Dose (MIRD) Committee of the Society of Nuclear Medicine; but the unabridged data included here and the beta spectra have not been previously published.

5. APPLICATION OF THE DATA
   This data base has been designed to address the needs in medical, environmental, and occupational radiation protection. Calculations of the spatial distribution of absorbed dose (depth-dose) requires information on the beta spectra, and these are compiled in a separate data file also included here. NUCDECAY is required by the CCC-620/SEECAL program to calculate age-dependent specific effective energies.

6. SOURCE AND SCOPE OF DATA
   The unabridged data used in preparing ICRP Publication 38 and a monograph of the MIRD Committee are distributed in electronic form in this package. The data are assembled in two collections. The collection referred to as ICRP38 consists of data on the energies and intensities of radiations emitted by the 825 radionuclides reported, although abridged, in ICRP Publication 38 plus an additional 13 radionuclides evaluated during preparation of a monograph for the MIRD Committee. The second collection, denoted as MIRD, contains data for the 242 radionuclides in the MIRD monograph noted above. Each collection consists of three ASCII files:
   (1) the index file (ICRP38.IDX or MIRD.IDX) is a sorted list of the radionuclides with pointers into the data files.
   (2) the radiation file (ICRP38.RAD or MIRD.RAD) contains data on the energies and intensities of the emitted radiations.
   (3) the beta spectra file (ICRP38.BET or MIRD.BET) contains the spectra for all beta emitters in the collection.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAM
   Four utility codes are provided. The code DEXRAX is used to extract the decay data from the library for radionuclide(s) specified for the user. The utility CHAIN lists the decay chain headed by a user-specified radionuclide. The RADLINE code identifies radionuclides which emit alpha or photon radiations of a user-specified energy. The executables and most of the source codes are provided. The Microsoft Fortran 5 compiler was used to compile the CHAINS code and the READDEC portion of the
DEXRAX code. The full source for DEXRAX is not provided as that implementation must be linked with two special libraries. The source code is provided for a QBASIC version of the utility RADSUM. This version of RADSUM does include plotting of the beta spectra or computations of the gamma constant. Other utilities were written in Microsoft BASIC Professional Development System.

8. DATA FORMAT AND COMPUTER
   ASCII; PC 386. (D00172/PC386/01)

9. TYPICAL RUNNING TIME
   The codes are interactive.

10. REFERENCES
    a. Documentation available with library
    b. Other useful documentation

11. CONTENTS OF LIBRARY
    Included are the referenced documents and two DS/HD 3.5-in. (1.44 MB) diskette written in compressed DOS files which include the data library, the installation code, and the utility codes.

12. DATE OF ABSTRACT
    November 1994; revised May 1995.

    KEYWORDS: BETA-RAY SPECTRA; MICROCOMPUTER; RADIOACTIVE DECAY SPECTRA; ELECTRON SPECTRA; EXTERNAL DOSE; INTERNAL DOSE; RADIONUCLIDES
1. NAME AND TITLE OF DATA LIBRARY
   RADDECY 4.02: Radioactive Decay Data for Radiological Assessments.

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS
   RADDECY 4.02 (DK4.EXE) - Display Decay Information of Radioactive Nuclides.
   MEV 1.03 Nuclide Search and Analysis Utility.

3. CONTRIBUTORS
   Original Contributor:
   Grove Engineering, Inc., Rockville, Maryland.

   Other Contributor:
   University of Connecticut, Storrs, Connecticut.

4. HISTORICAL BACKGROUND AND INFORMATION
   The data are derived from DLC-SODRALIST, a data set giving radioactive decay energies, spectra, half lives, and other information. RADDECY 4.02 is an interactive program for the IBM PC, or compatible, for retrieving and displaying decay information for 497 radionuclides. Data provided include the half life, radioactive daughter nuclides, probabilities per decay, and decay product energies for alpha particles, beta rays, positrons, electrons, x-rays, and gamma rays.

5. APPLICATION OF THE DATA
   The estimation of radiation dose to man from either external or internal exposure to radionuclides requires a knowledge of the energies and intensities of the atomic and nuclear radiations emitted during the radioactive decay process. The availability of evaluated decay data for the large number of radionuclides of interest is of fundamental importance for radiation dosimetry.

   The library includes radionuclides occurring naturally in the environment, those of potential importance in routine or accidental releases from the nuclear fuel cycle, those of current interest in nuclear medicine and fusion reactor technology, and some of those of interest in the estimation of annual limits on intake via inhalation and ingestion for occupationally exposed individuals.

6. SOURCE AND SCOPE OF DATA
   The radioactive decay data in the library were published in DOE/TIC-11026 (see reference below) and made available as DLC-80/DRALIST in the MEDLIST format.

   In addition to the radionuclides of interest in the nuclear fuel cycle, the data base comprises most of the nuclides occurring naturally in the environment, those of current interest in nuclear medicine and fusion reactor technology, and some additional radionuclides of use in the estimation of annual limits of intake and derived air concentrations for occupationally exposed individuals. The current data base contains approximately 500 radionuclides. It is believed that, with few exceptions, the decay data contained in this report are not likely to change significantly over the next few years as the result of new measurements.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAMS
   RADDECY (DK4.EXE) is a program for the IBM PC and compatibles for the retrieval and display of the decay information of radioactive nuclides. It is written in TrueBasic and compiled.
executable program is on the distribution diskette. The data are in a special format for retrieval by RADDECY which is defined in the documentation. A math co-processor is desirable but not necessary. The data files can be "exported" to an ASCII format. A search routine allows finding the radionuclides that have photon decay in a user specified energy range.

At the University of Connecticut the MEV Search and Analysis program was developed to assist in the identification of nuclides producing a spectrum on their Multi Channel Analyzer. MEV will search through either Alpha, Beta, or Gamma libraries for single energy line or for a group of energy lines. Each energy line is described by a specific energy in Mev, an uncertainty above and below this value to extend the search through, and a probability lower limit of yield to discriminate out low probability energy lines. Single energy line searches will result in a list of possible nuclides. Multiple energy line searches of up to six lines provide a list of possible nuclides and how many energy lines each nuclide matched. Also available is an option to display all the energy lines of any nuclide.

8. DATA FORMAT AND COMPUTER
   Executable and coded data files on one DS/HD 3.5-inch diskette (1.44 MB); IBM PC.

9. TYPICAL RUNNING TIME
   Interactive.

10. REFERENCES
    a. Included in package:
    b. Background information:

11. CONTENTS OF LIBRARY
    Included are the documents in 10.a. and one 3.5-in. (1.44 MB) DS/HD diskette written in DOS format which contains the data files and executable file and MEV program.

12. DATE OF ABSTRACT

    KEYWORDS: RADIOACTIVE DECAY SPECTRA; MICROCOMPUTER
1. NAME AND TITLE

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS
   FIXISO: To update the gamma-ray data file ordered by nuclide number.
   DECAYDAT: To read and list the gamma-ray data file ordered by nuclide number.
   NUCLIDE ID: To display data for a particular nuclide or list nuclides which emit gamma rays in a narrow energy range (IBM PC).
   TPASLIST: To read and list data file ordered by energy.

3. CONTRIBUTORS
   Oak Ridge National Laboratory, Oak Ridge, Tennessee.
   EG&G Energy Measurements, Inc., Goleta, California.

4. HISTORICAL BACKGROUND INFORMATION
   The data reported in DLC-19/DECAYGAM were the parent data for this library. Additions and changes have been primarily for fission product radionuclides and for heavy actinides. Other changes include determining the absolute normalization for most of the relative branching ratios given in the parent file.
   The original data library was made available April 1982. A major revision was made August 1983, another in September 1984, and another in October 1985.

5. APPLICATIONS OF THE DATA
   This compilation of radionuclide decay data contains, for those radionuclides tabulated, all necessary data for qualitatively and quantitatively measuring the concentration of photon emitting radionuclides as well as conducting activation analyses using gamma-ray spectrometry. It was developed specifically for use with RSICC code package PSR-164/TPASS.

6. SOURCE AND SCOPE OF DATA
   The TPASGAM data library contains gamma-ray decay information for 1438 radionuclides. The data consist of gamma-ray energies and intensities as well as cross-section information useful in activation analysis.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAMS
   D00088ALLCP04
   FIXISO, the program for editing the data library ordered by nuclide number, is an interactive PDP-10 Fortran IV program. The user is prompted to name the data file, to identify the nuclide to be edited and then for the datum to be replaced and its new value. More than one element may be changed while executing the program; however, the changes must be ordered by nuclide number since the input file is not rewound.
   DECAYDAT runs on the IBM 3033 and reads the data library ordered by nuclide number from unit 5 and prints it on unit 6 with comments.
   TPASLIST runs interactively on Vax computers. It reads the file ordered by energy and lists data for selected nuclides.
SEARCH.FOR is a Fortran program to perform searches for records on the data library ordered by nuclide number. It can be linked with additional subprograms to perform calculations required for user's applications.

**D00088IBMPC03**

NUCLEIDE ID is a compiled IBM PC program which displays data for a particular nuclide or lists nuclides which emit gamma rays in a specified energy range. The program is interactive. The data are stored in dBase III DBF format.

8. **DATA FORMAT AND COMPUTERS**

   EBCDIC card images; FIXISO, PDP-10; DECAYDAT, IBM 3033; TPASLIST, VAX.
   ASCII files of the nuclide ordered table; dBase III DBF files for NUCLIDE ID, IBM PC.

9. **TYPICAL RUNNING TIME**

   Several changes to the data file can be made running FIXISO in less than 15 CPU seconds.
   DECAYDAT runs in less than 3 CPU seconds.
   NUCLIDE ID is interactive.

10. **REFERENCES**

   a. Included in package:
      J. K. Dickens, Informal Notes (October 1985).

   b. Background information:
      RSICC Data Package DLC-19/DECAYGAM.

11. **CONTENTS OF LIBRARY**

   Included are the referenced document (a) and a reel of magnetic tape which contains three Fortran programs and the three data libraries ordered by nuclide number, energy and half life written in EBCDIC card images; total records 20,479.
   ASCII files (PC-DOS) for IBM PC (1 5.25-in. diskette). DBF files for IBM PC (3 5.25-in. diskettes).

12. **DATE OF ABSTRACT**


   **KEYWORD:** RADIOACTIVE DECAY SPECTRA
1. NAME AND TITLE OF DATA LIBRARY
   XG-IAEA: X-ray and Gamma-ray Standards For Detector Calibration

2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS
   XG: Executable X-Ray and Gamma-Ray DBASE program.

3. CONTRIBUTOR
   International Atomic Energy Agency, Vienna, Austria.

4. HISTORICAL BACKGROUND AND INFORMATION
   IAEA established a Coordinated Research Program (CRP) on the Measurements and Evaluation of
   X- and Gamma-ray Standards for Detector Efficiency Calibration in 1986 with the aim of alleviating the
   generation of data discrepancies. Representatives of nine research groups and one international
   organization performed precise measurements and systematic in-depth evaluations of the required decay
   data. They have also contributed to the development of evaluation methodology and measurement
   techniques and stimulated a number of such studies. Results of the work finished in 1990 are
   incorporated in XG-IAEA data base.

5. APPLICATION OF THE DATA
   Values of half-lives and photon emission probabilities are given for a selected set of radionuclides
   that are suitable for detector efficiency calibration.

6. SOURCE AND SCOPE OF DATA
   Data were evaluated from the open literature and laboratory reports published over a considerable
   period of time. The eventual omission of individual values had to be justified on the basis of their
   quality or other specific grounds. An evaluation procedure was developed for the half-life data. This
   procedure was also applied to the gamma-ray emission probabilities whenever appropriate. Included for
   36 selected radionuclides are three tables of recommended evaluated values and uncertainties of their
   half-lives; energies and emission probabilities of X-rays, energy range 5-90 keV; energies and emission
   probabilities of gamma-rays, energy range 14-3600 keV.

7. DISCUSSION OF THE DATA RETRIEVAL PROGRAMS
   The file XG.EXE is a DBASE program. At the PC prompt, one need only type XG. The data are
   shown in either nuclide sort or energy sort.

8. DATA FORMAT AND COMPUTER
   The data files are in DBASE format; IBM PC.

9. TYPICAL RUNNING TIME
   None noted.

10. REFERENCES
    H. D. Lemmel, "X-ray and Gamma-ray Standards for Detector Calibration," IAEA-TECDOC-619
    (September 1991).

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11. CONTENTS OF PACKAGE
The package contains the documents referenced, and an executable DBASE program and binary DBASE data files are transmitted on one DS/HD 5.25-inch diskette (1.2MB).

12. DATE OF ABSTRACT

KEYWORDS: MICROCOMPUTER; RADIOACTIVE DECAY SPECTRA
ACKNOWLEDGMENTS

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