Computer Code Abstracts

GSSLRN-I

An Automated Least-Squares Computer Code for the Analysis of Photopeak Spectra

1. Name of Code: GSSLRN-I
2. Computer: GSSLRN-I is designed to operate on the UNIVAC 1108 computer. Approximately 65 K words of directly addressable core are required.
3. Problems Solved: GSSLRN-I is utilized for evaluations and statistical determination of photopeaks in photon spectra. The code performs evaluations of photopeak spectra using as input the digitized pulse height distribution which is output from a large multichannel analyzer. Photopeaks are located, functions are fit to each real peak, and the relative intensity of each fitted peak above the background continuum is calculated. The code is easily adaptable for analysis of any spectra which can be adequately defined by peaks represented in analytic form. Thus, it is useful for application in such areas as: radiochemical analyses, analysis of reactor fuel burnup, half-life determinations, geological evaluations with respect to mineral content or time periods, analysis of Mossbauer spectra, and determination of elements in blood or body tissue.
4. Method of Solution: The code is based upon least-squares fitting techniques utilizing second-order Taylor's expansions with regression analysis. Varied tests have been incorporated into the code which rely on measurement variance, regression analysis, and deviation from a least-squares fit in order to effectively resolve multiplets in complex photopeak spectra.
5. Restrictions on the Complexity of the Problem: The number of channels from a multichannel analyzer, which can be analyzed per case, is limited to 2048. The total number of fitted peaks per case is limited to 200. The total number of channels per interval of fit is limited to 250. The total number of peaks per interval of fit is limited to 10. The code is limited to 49 parameters per interval of fit. The limits described above are based upon an analysis of photopeaks described by symmetric Gaussian analytical form.
6. Typical Machine Time: (Times quoted are for the UNIVAC 1108.) Running time varies from 2 to 6 sec per fitted peak and is a function primarily of the options of the code which are exercised. A typical problem would be the analysis of fission product spectra obtained from gamma-ray analysis. A problem of this nature would contain approximately 30 to 50 peaks and would require approximately 2 min of computer time.
7. Unusual Features of the Program: The code uses the fitted measurement variance in its decision analysis to decide if deviations from the fit are supported sufficiently to warrant a recycling attempt with higher groups of Gaussian terms so as to define hidden photopeaks. In the case of recycled multiple fitting, recovery procedures are engaged to supply the user with the last good fit which was obtained. The code has automatic plotting features to display the measured data, the fitted curve, and the root-mean-squared deviation envelope, in addition to displaying each resolved peak.
8. Related and Auxiliary Programs: GSSLRN-I requires the use of NAMELIST, a generalized input routine. The need for NAMELIST can be eliminated by substituting a comparable generalized input routine available at the particular site.
9. Status: GSSLRN-I is in production use on the UNIVAC 1108 computer at Pacific Northwest Laboratory, Richland, Washington.
10. Machine Requirements: Approximately 65 K words of directly addressable core storage are needed by the program. By reducing the maximum limits of the code it would be possible to scale the code down to fit on smaller machines. Approximately 131 000 octal locations of scratch drum storage are needed. Two tapes are needed in addition to the card reader, printer, and card punch. A Calcomp plotter is required to exercise the plotting options of the code.
11. Programming Language Used: The program is entirely in FORTRAN-V, with the exception of two minor machine language routines. These machine language routines could be eliminated and cause the loss of only one minor plotting option of the code. Programming of the code in FORTRAN-IV would require only minor effort.
12. Operating System: UNIVAC 1108 computer with FORTRAN-V compiler and CSCX operating system. The Calcomp plotter model 763 is used for the plotting options.
13. Programming Information: GSSLRN-I consists of 50 subroutines using about 4000 source cards. The program presently uses an overlay structure consisting of the main link and five overlay segments.
14. User Information: The code and report may be obtained either through the Argonne Code Center at Argonne National Laboratory or from Pacific Northwest Laboratory in Richland, Washington.
15. *Acknowledgment:* This paper is based on work performed under U.S. Atomic Energy Commission Contract AT(45-1)-1830.

16. *References:*

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[2]BERNARD H. DUANE, "Maximum Likelihood Nonlinear Correlated Fields (BNW Program LIKELY)," USAEC Report, BNWL-390, Pacific Northwest Laboratory (1967).

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RICE

1. Name of Code: RICE
2. Computer for Which Code is Designed: RICE is written to operate on computers in the IBM-360 series.
3. Problems Solved: The program calculates an energy exchange matrix which describes the probability that a neutron with energy E will produce a recoil atom with energy T in a given material. In addition, the program can calculate the primary recoil atom energy spectrum for a given neutron spectrum, the damage cross section for the material, and an optimum lower energy limit for use in comparing the relative damage in different reactor spectra. The program accepts neutron scattering data directly from the ENDF/B library tapes and, in the case of a resonance nuclide, from a tape generated by the program SUPERTOG.
4. Method of Solution: The energy transfer matrix is obtained from a solution of the two body kinematic equations. The solution incorporates information on anisotropic elastic scattering and inelastic scattering available from ENDF/B. Damage cross sections and primary recoil spectra are obtained by combining the energy transfer matrix with suitable secondary displacement models and neutron flux spectra.
5. Restrictions on Complexity of the Problem: RICE does not recognize all of the multiplicity of data formats allowed by ENDF/B. It is programmed to accept the most prevalent formats. These restrictions are described in detail in the program manual. In addition, the neutron energy distribution is restricted to a 99-group representation and the recoil energies are represented by 200 energy groups.
6. Typical Machine Time: Running time on the IBM 360/75 for one element with all options requested is approximately 10 min.
7. Unusual Features of the Program: The inclusion of inelastic scattering in the calculation of recoil spectra and the ability to work directly from ENDF/B format tapes are both features previously unavailable in this type of program.
8. Related and Auxiliary Programs: RICE lacks the capability of calculating elastic scattering cross sections from resonance parameters. The code SUPERTOG (ORNL-TM-2679) can be used to produce smooth elastic scattering cross sections for RICE in cases where resonance parameters are included in the ENDF/B data. The multigroup programs GAM-II, ANISN, and XSDRN can be used to produce neutron spectra for use in RICE.
9. Status: RICE is in production use on the IBM 360/75 and 360/91 at the ORNL Computing Center.
10. Machine Requirements: Approximately 110 000 words of core storage and five I/O devices excluding input-output and system requirements are needed by the program. A plotting routine makes use of ORNL system subroutines and a Calcomp CTR plotter.
11. Programming Language Used: The program is written in FORTRAN IV.
12. Operating System: IBM OS/360 with the FORTRAN H compiler.
13. Programming Information: The program presently consists of about 3000 FORTRAN statements in 45 subroutines.
14. Users Information: The code and report may be obtained either through the Argonne Code Center at Argonne National Laboratory or through the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory.
15. *Acknowledgment:* This research was sponsored by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation.
16. *Reference:*

J. D. JENKINS, "RICE: A Program to Calculate Primary Recoil Atom Spectra from ENDF/B Data," ORNL-TM-2706, Oak Ridge National Laboratory (1970).

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