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Reaction Rates in SAIPS. Part 2: Software and
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METHODS OF NEUTRON SPECTRUM CALCULATION FROM MEASURED
REACTION RATES IN SAIPS. PART 2: SOFTWARE AND
DATA INPUT

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During the All-Union School on the Metrology of Neutron Measurements in Nuclear Physics Facilities at Riga in 1976 the need for a library of programs for calculating neutron spectra from measured reaction rates was recognized, and it was decided to establish such a library. The unfolding of neutron spectra is performed by non-identical mathematical methods taking the form of various programs and some neutron cross-section libraries. The physicist-user needing to perform calculations faces a number of problems: obtaining or writing the programs, comparing them, obtaining the necessary cross-sections, establishing the required cross-section library, establishing a library of reference spectra, investigating the calculated spectrum, and so on. As a result, routine work is duplicated by many laboratories. The information processing system SAIPS, some aspects of which are described in Refs [1, 2], was created for the solution of these problems. Our paper gives a brief description of the SAIPS software and the basic principles of its application.

SAIPS was produced on the ES 1022 computer under the control of the operational system OS ES version 4.1. SAIPS contains programs needed to unfold spectra, libraries of neutron cross-sections and reference spectra, and software for automatic calculation and for system maintenance. With SAIPS a calculation method can be perfected, in particular, for determining the reliability of a spectrum obtained and for planning reaction rate measurements.

1. The programs SAND-II [11, 22], WINDOWS [24], RFSP JÜL [14] and PM [4] have been incorporated in SAIPS, adapted and tested and are available for use in calculations. SAIPS contains several more programs (see Table 1) which can be used in calculations, but they duplicate the programs listed above, and are more limited. These programs include: CRYSTAL BALL [19], the solving method of which is borrowed in WINDOWS; SPECTRA [15, 16]; RFSP [9] and GIN [6], which use the same solution algorithm as that used, in a more developed form, in RFSP JÜL; and LIKMET, a program using the maximum likelihood method (MLM) [8]. Table 2 presents data on the computing resources used by the recommended programs. The calculating time was determined for a system with 11 detectors. The criterion for completion of a calculation in all programs was selected such that the calculated activation integrals did not differ from the given integrals by more than 5%. "Astronomical time" is the calculating time in a single-program regime. "Commercial time" is the "charge" for the computing resources drawn upon by the programs: central processor time, internal memory capacity, the extent to which peripheral equipment is used, etc. All programs except PM are written in FORTRAN IV. For this reason the internal memory capacity taken up by the programs depends on the maximum size of the data provided. This disadvantage was avoided by using the PL/1 language to write the PM program. The high level of compatibility of both hardware and software between the third-generation ES EhVM and IBM computers made it possible to adapt the unfolding programs and to use them without modification in calculations. In addition, modified versions were prepared in which the data output was changed. The results obtained are first recorded in an intermediate set of data from which they are then converted into the required form.

So far the following cross-section libraries have been adapted for SAIPS: ENDF/B-IV [21] and ENDF/B-V [20]; the dosimetric file ZACRSS [3]; BOSPOR 78 [7]; libraries supplied with programs: SAND-II (a library known as CCC112B and, in a modified version, DETAN 74 [23]); WINDOWS, RFSP JÜL and some individual cross-sections. Altogether SAIPS contains cross-sections for more than 80 reactions used in unfolding. In performing calculations it is possible to use the spectra libraries of the SAND-II program from Refs [5, 18] as a first approximation.

2. Using SAIPS for his calculations releases the user-physicist from the need to go into questions of programming. With this in view we suggest dividing work with SAIPS into three levels, each supported by its own software.

Level 1: This level involves adapting, writing, testing and examining the programs and the libraries of cross-sections and spectra; preparation of the software for automatic calculations, use of the libraries of cross-sections and spectra, updating and further development of the system; issuing of the distribution version of the system, etc. The work is done centrally, to avoid duplication in several laboratories and to save the user-physicist unnecessary routine labour. Work on this level is carried out by programmers with the assistance of physicists.

Level 2: At this level SAIPS is used in the actual computing environment. The SAIPS control program occupies up to 150 kilobytes of internal memory. The distribution version contains loading program modules, neutron spectra libraries, and a library of catalogued procedures. Level-2 work is performed by computer staff using the standard resources of the operational system.

Level 3: This level corresponds to the performance of calculations. The user addresses the system in user's language and with statements in the OS ES problem control language. The set of catalogued procedures of SAIPS simplifies access to the system. The user's language is based on the terminology used in this application. No effort to learn it is therefore required. Using SAIPS, it is possible:

- to have a uniform input of initial data and output of results for various methods of calculation;
- to reduce the number of parameters introduced;
- to vary cross-section libraries and individual cross-sections;
- to take into account the presence of one or more absorbers covering the detectors;
- to introduce an a priori spectrum from the incoming flux or to select one from the library indicated or to pick the most suitable one from that library by the least-squares method.

3. SAIPS offers the possibility of determining the reliability of an unfolded neutron spectrum and of planning measurements and calculations by varying different factors: the errors in the reaction rates, the errors in the cross-sections used, the detector assembly, the a priori information, the unfolding programs, etc. The information content and description provided by the system are such that the user can perform these calculations without much effort. Note that comparisons performed to study such questions in view of incorrect definition of the problem can be generalized with great care. After examining the physical conditions determining the formation of the neutron spectrum to be unfolded, it is necessary to present the a priori information concerning the spectrum. Usually this a priori information is a first approximation in spectrum unfolding programs. In the stage of planning for a previously determined neutron spectrum the influence of the factors listed above is studied. The requirements imposed on the neutron spectrum to be unfolded determine the detector assembly, the accuracy of measurement of the reaction rates, the permissible uncertainty in the a priori information, etc. After unfolding, similar calculations are carried out to determine the error in the neutron spectrum obtained. The actual steps taken in each case depend on the requirements with respect to unfolding, previous experience, etc. The method presented here entails a high cost in computing resources, but in view of the incorrect nature of the problem to be solved it is often impossible to get by without such calculations.

CONCLUSION

A large set of cross-section and spectrum libraries etc. in effect constitutes an "information burial ground". Although the information is there, the user may be unfamiliar with it and must therefore make an independent assessment of its value, create the means of using it, and so on. The development of systems like SAIPS brings about a qualitative change in the relationship between the information and the user, since such systems provide the means of using the information as well as the information itself.

Further development of SAIPS will involve the combination of a larger range of programs and input data for calculations of neutron spectra. To this end we are adapting the cross-sections of the whole ENDF/B-IV file, obtained from the IAEA, the cross-section library processing program AMPXII [17], and the programs ANISIN [13] and MORSE [12] obtained from the Radiation Shielding Information Center (RSIC), Oak Ridge, USA.

Table 1
SAIPS unfolding programs

Name of program	Unfolding method	Type of computers on which programs are run	Number of energy groups or points	Maximum number of detectors	Source	Remarks
SAND-II	SAND-II	IBM/360 ES EhVM CDC 6600	620	35	RSIC	
MPS	MMP and SAND-II	ES EhVM	620	35		Obtained by modifying SAND-II program
CRYSTAL BALL	CRYSTAL BALL	IBM/360 ES EhVM	621	20 or 40	RSIC	
WINDOWS	CRYSTAL BALL	IBM/360 ES EhVM	621	15 or 40	RSIC	In this program the CRYSTAL BALL method is perfected and further developed.
SPECTRA	SPECTRA	CDC 6600 ES EhVM	up to 100	30	RSIC	A program adapted for ES EhVM and translated into PL/1.
RFSP	SPECTRA	ICT-1905	up to 50	30	Author	Based on SPECTRA program.
RFSP JÜL	SPECTRA	IBM/360 ES EhVM	up to 100	30	RSIC	Based on RFSP and SPECTRA programs.
GIN	SPECTRA	ES EhVM	100	30	Author	Based on RFSP and SPECTRA programs.
PM	Polynomial method	ES EhVM	Indicated by user.		Our own development	Program written in PL/1 so that memory can be used dynamically.
OBR 30	Statistical regularization [10]	BEhSM-6 ES EhVM	100	20	Author	Modification of a program written for unfolding neutron spectra at Moscow Engineering and Physics Institute.

Table 2
Computing resources used by calculation programs

No.	Name of program	Calculating time (min)		Internal memory occupied (kilobytes)
		Astronomical	Commercial	
1	SAND-II	2.5	6.5	112
2	PM	1.7	4.5	136
3	RFSP JÜL	12.7	21	234
4	WINDOWS	2	5	248

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