A PROGRAM FOR CALCULATING GROUP CONSTANTS ON THE BASIS OF LIBRARIES OF EVALUATED NEUTRON DATA

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ABSTRACT

The GRUKON program is designed for processing libraries of evaluated neutron data into group and fine-group (having some 300 groups) microscopic constants. In structure it is a package of applications programs with three basic components: a monitor, a command language and a library of functional modules. The first operative version of the package was restricted to obtaining mid-group non-block cross-sections from evaluated neutron data libraries in the ENDF/B format. This was then used to process other libraries. In the next two versions, cross-section table conversion modules and self-shielding factor calculation modules, respectively, were added to the functions already in the package. Currently, a fourth version of the GRUKON applications program package, for calculation of sub-group parameters, is under preparation.

The GRUKON (group constant calculation) program is part of the system for supplying constants for nuclear reactor and radiation shielding calculations (SOKRATOR) [1]. The GRUKON program, along with the FOND library of evaluated neutron data files [2], forms the MIKRO sub-system, which is designed to generate periodically, for a given set of nuclides, multigroup and fine-group constants (having, respectively, several tens and several hundreds of groups), independently of the composition of the medium. As an example, we may cite the well-known BNAB system [3] and also the MUL'TIK system of 250 groups (in the slowing-down region), which is currently being developed for checking multigroup approximations [4].

In structure, GRUKON is a package of applications programs [5] whose basic components are:

- A set of functional modules which carry out various structural conversions on neutron cross-section data;
- Systems software to sequence processing by the functional modules (according to task) and to provide information links between modules;
- A command system by means of which the user runs the data structure conversion program.

Data exchange between the functional modules is by standard information units (standard representations) which are stored in the package's working library, or standard representations library (BSP). The GRUKON package of applications programs can thus be described as a program package with standard function loading. A description of the package hardware and capabilities and of its operating instructions is contained in Refs [6-9].

Structure of the function loading

All conversions carried out by GRUKON can be divided into four groups:

- Data input from punched cards or from evaluated data libraries, converted into standard form and entered in the BSP;
- Algorithmic conversions, which switch from one method of representing cross-section data to another;
- Editing conversions, which change only the locations of data within the BSP without altering the internal structure of the standard representations;
- Output of data from the BSP, i.e. to an alphanumeric printer in the form of lists or annotated tables, or converted into group constant library format and entered in the device indicated.

The second group of conversions being the more important, we shall examine it in greater detail. The conversions in this group are chosen in such a way as to facilitate the transition from the representation of cross-section data used in the evaluated data libraries to the representation

of data as constants. As we know, the evaluated data libraries represent cross-section resonance structure by means of resolved resonance parameters (R), tables of cross-section energy dependences (S) and mean resonance parameters (U), whereas cross-section group functionals (F) and sub-group parameters (P) are characteristic of group constant libraries. The problem is thus how to make the transition from the R, S, U set to F or P representation. In the GRUKON package this transition is accomplished by the following modules:

- Calculation of the detailed cross-section behaviour from the resolved resonance parameters (R/T-S);
- Calculation of the cross-sections for a given temperature (S/T-S);
- Calculation of the energy dependence of the expected values of the cross-section functionals on the basis of the energy dependence of the mean resonance parameters (U/D-F);
- Addition of various cross-section components given by the detailed behaviour and reduction to a general set of fundamental energies (S/C-S);
- Computation of group functionals on the basis of the detailed cross-section behaviour (S/G-F);
- Computation of group functionals on the basis of the energy dependence of the expected values of the cross-section functionals (F/G-F);
- Convolution of the cross-section functionals given for the various components of the cross-sections (F/C-F);
- Obtaining of sub-group parameters on the basis of the dependence of the cross-section group functionals on the cross-section environment, dilution and temperature parameters (F/-P).

The conversion system is shown in Fig. 1. The special feature of this system is that it does not involve the limitations usually applied by processing programs to evaluated data libraries, namely (1) that the total

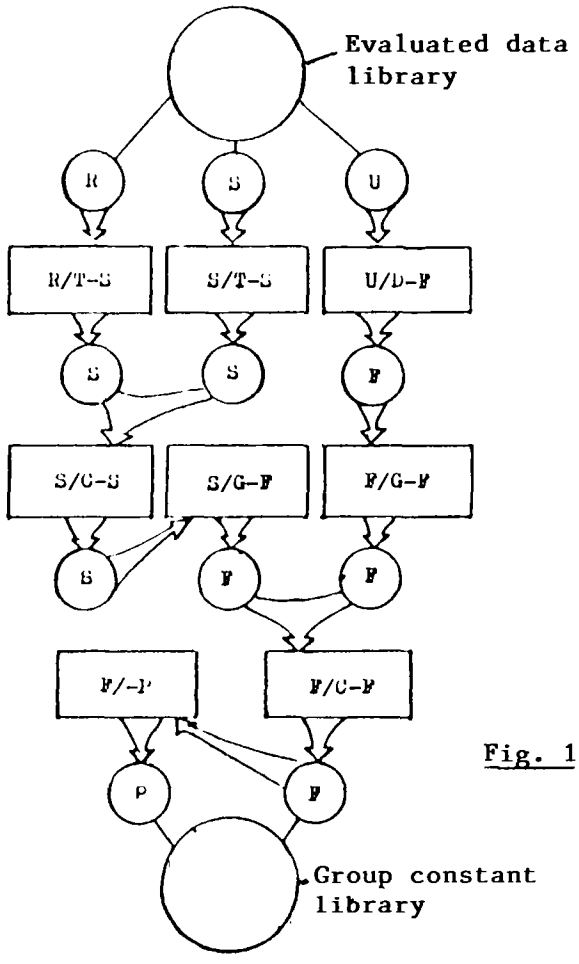

Fig. 1. System for converting evaluated neutron cross-section data into group constants

cross-section must be given for a set of fundamental energies representing a combination of all sets for national cross-sections; and (2) that the resolved and unresolved resonance regions must not overlap, even if the resonances are related to different systems [10]. This feature increases the system's ability to represent cross-section resonance structure in evaluated data libraries.

At present, the capabilities of the GRUKON applications program package's loaded functions are greater than required to solve the basic problem. It has been found that these are closely related problems which can be solved to some extent using the existing functional modules, such as analysis of microscopic experiment data, evaluation of neutron cross-sections and generation of evaluated data libraries. However, it was considered useful to expand the set of modules so as to cover these areas more fully. For example, a group of modules for converting cross-section tables has appeared

which is designed to automate the generation of detailed cross-section behaviour files, and the capabilities of the S/G-F, U/D-F and F/C-F modules were increased so that experimentally measurable transmission and self-indication functions could be calculated as well as the block cross-sections used in group constant libraries.

Currently, the total number of functional modules (including the input/output and editing modules) is 28 [9].

Conversion control and data exchange organization

There are two levels of data conversion control in the GRUKON package. The first level of control uses what is termed a conversion program, fed in from punched cards at the beginning of the calculation by the monitor program of the package (Fig. 2). The conversion program uses stationary language (see below) to establish the sequence in which the functional modules are called up and to determine the location of data in the BSP.

The second control level - control of module operating mode - uses "conversion parameters". The parameters are entered from punched cards by the INPUT module and stored in the BSP along with the basic cross-section data, from which they differ only in name (both the basic data and the parameters have the same formal structure of standard representations. As the set of parameters is specified for each module, their conventional names coincide with the names of the corresponding conversions. For example, in the case of the module for calculating detailed behaviour from resonance parameters (R/T-S), the conversion parameters are named R/T-S and contain the number of the resonance formula, the numbers of temperatures for which the cross-sections must be computed, the energy interval boundaries, the accuracy of interpolation between fundamental energies, and temperature values. All data entered into the BSP (irrespective of whether they are external input or the results of calculations) are logged by the monitor program in the BSP catalogue, in which are entered: the data name, the number of the device in

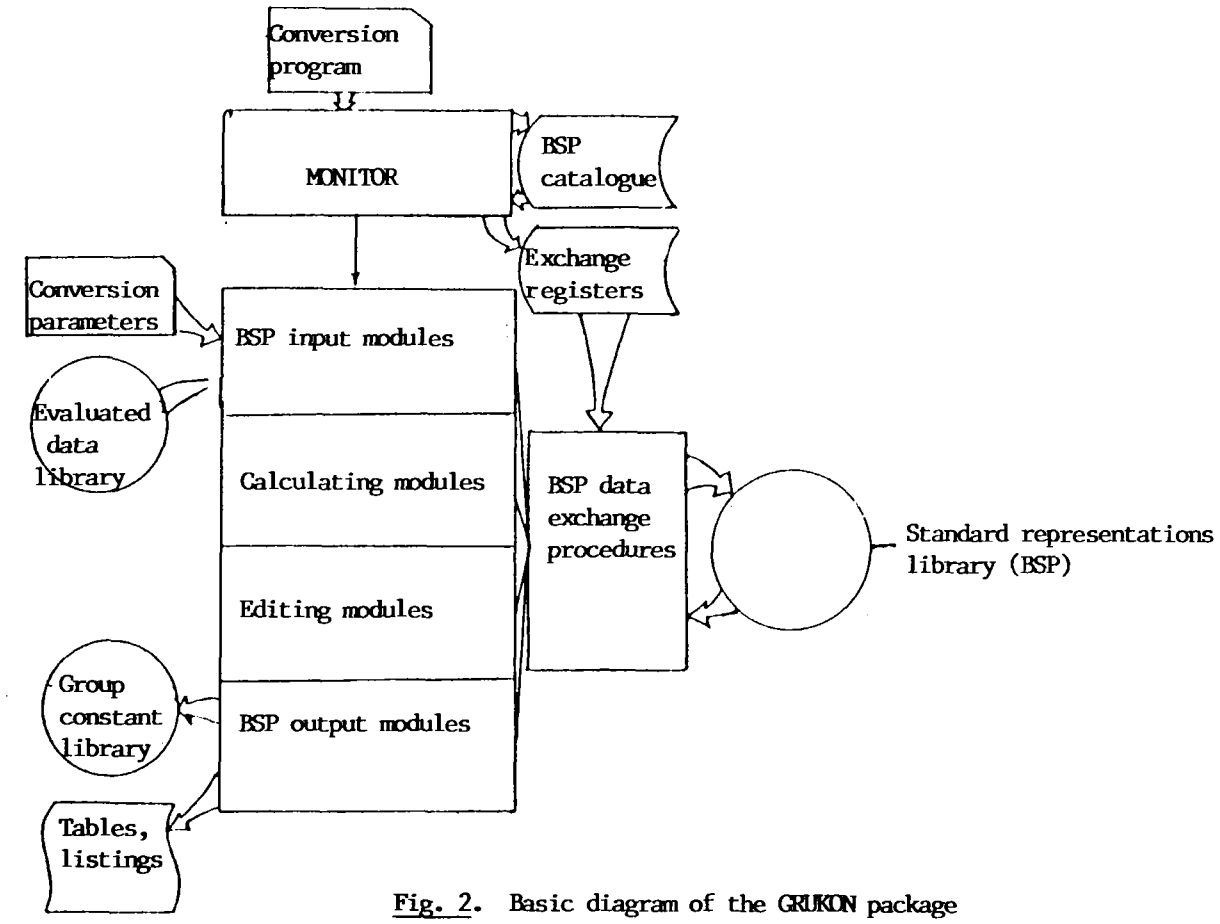

Fig. 2. Basic diagram of the GRUKON package

which they are stored, the initial address of the data, and their length (in words). Before calling up the next module, the monitor program analyses the next command in the conversion program, determines the address of the source data to be used in the conversion and builds up exchange registers from them. In this way the system exchange procedures used in the telefunctional modules for reading and writing data from the BSP are adjusted to a particular operating mode. Information on the location of data is thus excluded from the telefunctional modules, which much simplifies programming them. At the same time, correct use of the systems procedures for data exchange with the BSP provides a data link between modules and protects the BSP. Information is exchanged between the modules and the BSP along three channels: the first carries source data, the second carries the parameters, and calculation results are recorded through the third. Information is fed through each of the channels page by page by way of the corresponding buffer arrays (sheets).

The devices to which the data channels are attached may be either the same or different; in the latter case, the page/channel correspondence is not observed and pages are exchanged taking the access frequency into account.

Command system

Four groups of commands are used in the conversion program:

- For data conversion (including input, output, editing and algorithmic conversions);
- For catalogue generation (enter in catalogue, alter data names and print out catalogue contents on alphanumeric printer);
- For designating the working field of the BSP library;
- For control (repeat command groups, end conversion).

The commands in the first group have the most general structure, so we shall confine our remarks to them. The conversion command has a three-address structure: I, J, K, <k-data name>, <k-data address in BSP>; where I, J and K are the addresses in the BSP catalogue of the source data, the parameters and the conversion results, respectively (data address in the catalogue means the number of the catalogue line on which they are recorded). Apart from data addresses, a comand may also indicate the name assumed by a conversion result and the address at which the data should be entered in the BSP (if the address is omitted, the results are entered in the BSP working field starting at the first free word). Address in the BSP means the device number, the number of the first word, and the number of words occupied by the data. Note that a need to indicate the BSP address does not often arise so the command structure is usually fairly simple. The remaining commands are a subset of the conversion commands; for example, the command to end conversion consists of one name, written ,,,END. There is a detailed description of the command system used in the GRUKON package in Ref. [6]. The return to "code programming" in the input language of the GRUKON package might appear to be a backwards step, unless it is taken into account that the appearance of

higher-level languages was related to the requirements of automated programming, which do not arise in this case.

Operating experience and prospects for program development

Since the first operative version of the GRUKON package was put on the BEhSM-6 computer, it has been used for the preliminary processing of data available to the author from foreign data libraries (the American libraries ENDL-78 [11] and ENDF/B-IV [12], some files of ENDF/B-V [13], and also the Japanese library JENDL-J [14] into 28-group non-block cross-sections averaged with standard spectrum weighting in the BNAB group division [3]. Cross-section evaluation calculations were carried out and detailed behaviour files were generated from the FOND evaluated data library.

Mid-group values for cross-sections were obtained for basic reactor materials using the 250-group MUL'TIK division, and work began on calculating the sub-group parameters. Currently, the algorithms for obtaining sub-group parameters are being run in, and work has begun on transferring the program to the ES-1060 computer. It is proposed in the immediate future to include in the package modules for processing data on neutron angular and energy distributions, functioning in an autonomous mode for the time being.

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