A technology for preprocessing of group macroscopic constants and a technique for their refinement during neutron transport problem computation


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The paper addresses a system of constant support of neutron-physical computations, in particular, the energy release computation in the group transport approximation, that has been developed by RFNC-VNIIEF. The idea of the system is using a closed processing chain of data manipulation: operation with libraries of evaluated neutron data, development of recommendations on using one or another library of constants for different problem classes, calculation of group constants, and refinement of the constants during solution of time-dependent neutron transport problems.

Introduction

The numerical simulation of neutron transport in material is one of major directions of computational physics. A most widespread approach to simulation of this process is a so-called group approach. The accuracy and reliability of its results is largely dependent on the “quality” (i.e. their correspondence with the physical process that occurs) of the group characteristics of interactions between neutrons and material nuclei, which are used in the transport equation solution, i.e. on the “quality” of the group neutron constants. So one possible method for enhancement of the accuracy and physical reliability of the neutron transport problem solution results is to enhance the “quality” of the group constants used during the problem solution, which is known to depend, in the main, on the following factors:

1) Correspondence of the source spectral data used for the group constant preprocessing (as a rule, from libraries of evaluated neutron data) to a specific problem to be solved or problem class;

2) Correctness of the choice of the group energy partition for the problem;
The group constant preprocessing method, which is determined by specific computational algorithms and proper choice of weight functions (which are typically unknown in advance) used in the computations.

The paper discusses the system of constant support of neutron-physical computations that has been developed by VNIIEF. The principal task, which to tackle the system has been just developed for, above all is a higher “quality” of the preprocessing of group macroscopic neutron constants and constants of $\gamma$-generation and $\gamma$-interaction. All the system components form a closed processing chain: involvement of libraries of evaluated neutron data, development of recommendations on using one or another library of constants for different problem classes, calculation of group constants, and refinement of the constants during solution of time-dependent neutron transport problems. At that step the principal efforts of the developers were directed toward development of methods, programs, and technologies of data manipulation (i.e. such components of the system), which would mitigate and, in the ideal case, remove errors at all that are introduced by two of the three above factors and deteriorate the “quality” of the group constants and, hence, the accuracy and physical reliability of the neutron transport equation solution results. The case in point is primarily the first factor (the correspondence of the source spectral data to the problem to be solved) and the third factor (enhancement of the group constant preprocessing quality through using “proper” weight functions, i.e. the ones corresponding to parameters of the system to be computed).

**General description of the constant support system**

The general scheme of the neutron-physical computation constant support system appears in Fig. 1.
Figure 1. General scheme of the constant support system

BEND

Bank of Evaluated Nuclear Data

Nuclear Data Information - Reference

Program Code

EXFOR

International library of experimental data

BEND

Bank of Evaluated Nuclear Data

Recommended data

BEAR

Bank of Benchmarks

GEMUS

Multigroup Constants Archive

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As seen from the above scheme, the basic components of the constant support system are:

(1) **Databases:**

- **International Library EXFOR** of experimental nuclear-physical data (the library description can be found, e.g., in McLane (2000)). Presently it contains over 103 000 electronic publications by different authors (more than 500 Mbytes). It is used mainly for comparative analyses of evaluated data from different sources;

- **Archive BEND** of libraries of evaluated nuclear data (Farafontov and Grebennikov, 1994). Presently it contains over 25 libraries of evaluated data from different nuclear centers of the world, with its total amount being 1.5 Gbytes of data;

- **Bank BEAR of Benchmarks.** In contains geometry and results of experimental measurements of some integral characteristics of over 300 spherical and cylindrical systems;

- **Archive GEMUS of multi-group neutron constants, γ-generation and γ-interaction constants.** Unlike the above-described databases produced from external sources, the archive contains systems calculated with the program complex of the group constant system, each of which is designed for calculation either of separate specialized problems or different (heat, fast, etc.) problem classes. Each of the systems contains group data of a certain isotope set from certain libraries of evaluated data prepared using a special energy partition, different special weight functions, certain grids in temperature dependence, in dilution cross section, etc. Presently the archive contains more than 300 specialized systems of constants.

(2) **Software:**

- **Program complex of Archive BEND** (Farafontov and Grebennikov, 1994). It is designed in the main for control, processing and computation of spectral data from libraries of group constants and for computation and control of group data;

- **Software used during solution of problems of neutron and γ transport for preprocessing of group macroscopic constants and for refinement of group data during the computation.**
Two points should be mentioned:

1. All of the above constant support databases are completed with graphic service shells that, first, control the stored data integrity, second, allow the tabular and graphic data representation in the user-friendly form, comparative analysis of different characteristics, including those from different databases;

2. The experimental data library EXFOR and the evaluated data library archive BEND as well as a number of databases on nucleus structure and nuclear-physical interactions (not shown in the figure) are immersed in information-reference nuclear data system NDX (Grebennikov et al., 2001). The system in essence is an automated workstation of the specialist in the area of nuclear-physical data. The NDX possibilities will be discussed in more detail below.

Briefly consider the principal components of the system and the basic approaches to the manipulation of nuclear constants.

**Archive of libraries of evaluated nuclear data and program complex for their manipulation**

Presently, the archive (Farafontov and Grebennikov, 1994) contains more than 25 libraries of evaluated nuclear data on interactions of neutrons, protons, deuterons, tritium, gamma radiation with matter from different nuclear centers of the world (the United States, Japan, China, Europe, Russia) as well as specialized libraries and libraries recommended for different problem classes that have been developed by VNIIEF. There are more than 9000 isotopes, the amount is 1.5 Gb. The format of US library ENDF (Rose and Dunford, 1976, BNL, 1997) is taken for the data storage format. The archive is arranged in the form of a three-level hierarchical structure ensuring a convenient and consistent access to different data classes (see Fig. 2).

The program complex of the archive BEND is designed both for the spectral data processing and group constant computation and for manipulation of previously calculated group constants. The complex programs are written in the Fortran-90 language, the total amount is about 100 000 lines. The approach implemented in software package NJOY of US Los Alamos National Laboratory (MacFarlane and Muir, 1994) is taken as a basis of the concept of the data manipulation. A number of codes manipulating spectral data from the NJOY package have been adapted to and included in the complex BEND. The major BEND codes execute:

- Structural and physical control of spectral and group data;
- Construction of spectral neutron cross sections from resonance parameters;
- Calculation of effective spectral data with account for medium nuclei motion and chemical bonds of atoms in materials;
• Calculation of integral quantities: resonance integrals, average cross sections in different spectra, Westcott’s G-factors, transmission function;

• Calculation of group neutron constants and $\gamma$-generation constants with inclusion of resonance self-shielding;

• Calculation of equivalent isotropic group constants;

• Calculation of characteristics of one-dimensional critical systems in the multi-group anisotropic approximation.

**Figure 2.** Hierarchical structure of archive BEND.

**Nuclear data information-reference system NDX**

Presently, in the area of the constant support of nuclear-physical computations quite a wide electronic source stock of various published nuclear data is available and used in practice. In their essence, the data can be both results of direct experimental measurements and estimates obtained from different theoretical models. International Atomic Energy Agency (IAEA, Vienna, Austria) is distributing both separate files with data describing the atomic nucleus structure and a variety of libraries of experimentally measured data, libraries of evaluated constants with information on elementary particle-nucleus interactions.
The practice of using various nuclear databases and their service software allowed us to formulate three key concepts of the further development of service constant support software:

1. Integration of different-purpose databases from different sources with the capability of their graphic comparative analysis within a single program shell;

2. The capability of the user’s analysis of the suitability of data from one or another source (given one-type data from different sources) for solution of the user’s problems;

3. Development of the shell, such as the information-reference system with a flexibly adjustable content and varied size of supplied databases oriented to demands of different user categories.

These theses just form the basis of the concept of the nuclear data information-reference system NDX (Nuclear Data Expert’s Studio) under discussion, which has been developed by RFNC-VNIIEF for provision of nuclear-physics specialists with all needed data represented in a user-friendly graphic form, with the capability of their processing and some analysis of their “quality” (Grebennikov et al., 2001).

Thus, the NDX system is integration under a single graphic shell of various data describing both the nucleus structure and characteristics of interactions of different particles and radiations with material nuclei and completed with mathematical apparatus for the stored data processing and analysis. The system has been developed using advanced programming technologies and is a convenient tool for specialists who pursue nuclear-physical data problems.

In the light of the aforesaid it follows that the information-reference system NDX can be viewed as a component of the computer automated workstation of the specialist in the area of nuclear-physical data.

The principal data types included in NDX

Presently, NDX includes the following data types of open and periodically published sources:

- Evaluated nuclear data on characteristics of interactions of particles and radiations with material nuclei in the format of archive BEND.

- International Library EXFOR of experimental data. It contains experimentally measured data on characteristics of nuclear processes in a special format from more than 103,000 publications in different world nuclear-physics journals;

- Data from the table of nuclear masses and reaction energies by Audi and Wapstra (1995);
• Data from the International Base ENSDF on atomic nucleus structure (Tuili, 1987), including: characteristics of excitation levels; parameters of gamma radiation yield levels; properties of the ground and metastable states; etc.

• Data of isotope properties Karlsruher Nuklidkarte (1995);

• Data on prompt fission products. Information about radioactive decays of fission products (Kolobashkin et al., 1969).

A separate talk should be devoted to the description of the principal NDX possibilities alone. So here we will briefly dwell only on the possibilities offered by the system in manipulation of the evaluated spectral data as most voluminous and most significant in practice for the constant support of nuclear-physical computations. The principal available capabilities are:

• Tabular scanning and construction of 2D and 3D graphs of different quantities, with the possibility to superimpose the dependencies on one graph for their comparison and comparison of them to the experimental data of the EXFOR library;

• Some computational capabilities of data processing: construction of point-by-point behaviors of cross sections of processes from resonance parameters, Doppler broadening of cross sections of processes for different temperatures of medium nuclei;

• Calculation of some integral characteristics, such as average cross sections of processes in different spectra (Maxwell, NBS, Watt spectra), resonance integrals, Westcott’s G-factors, etc. These integral quantities can be used to assess the quality of the evaluated data from one or another source by their comparison to published or experimental values. Besides, the computed resonance integrals and values at thermal point can be compared to the associated values from the ENSDF base.

Fig. 3 gives examples of the evaluated spectral data manipulation.
Figure 3. Examples of the graphic representation and analysis of evaluated spectral and experimental data in the NDX system.
The principal approaches to assessment of the “quality” of evaluated spectral constants and development of recommendations on their application

As mentioned above, one of the basic reasons deteriorating the physical reliability of the transport equation solution results is the incomplete correspondence of the neutron-nuclear constants used to a specific problem being solved or problem class. Term it the degree of the data applicability for solution of a specific problem. It is our view that at the moment there is no single, universal neutron constant library applicable for solution of all problem classes faced by us.

RFNC-VNIIEF has adopted an approach, which consists in development of specialized libraries of constants recommended for calculation of certain problem classes on the basis of available data in the world libraries of evaluated constants and their partial modification.

The process of assessment of the “quality” of data or, more precisely, their applicability for certain problems and development of recommended libraries consists of several steps:

(1) Comparative analysis of data from the considered libraries of evaluated constants to experimentally measured data (the library EXFOR). Most representative characteristics and processes on the entire set of isotopes under consideration are analyzed;

(2) Comparison of calculated integral characteristics (average cross sections in different characteristic spectra, resonance integrals, Westcott’s G-factors, etc.) to experimental or recommended data;

(3) Calculations of parameters of critical assemblies simulating a certain problem class. For example, during the development of one of the recommended production libraries about 100 critical assemblies were calculated.

On analysis of the results of these three steps, a decision is made regarding inclusion of an isotope from one or another library in the recommended library being developed for a given problem class on the basis of expert judgement. Sometimes decisions of slight modification of the data to be included are made. For instance, one of the above-mentioned recommended libraries for solution of transmutation problems contains data for 97 isotopes from 6 world libraries, 4 isotopes have been obtained with VNIIEF techniques and programs.

Refinement of group constants during the process of the neutron transport problem solution

The existing technology for the preprocessing of group constants for the neutron transport equation solution appears about as follows:

(1) Assessment of applicability of neutron-physical characteristics of isotopes from different libraries of evaluated data for calculation of a certain problem class (as discussed above);
Selection of the group energy partition. This step of the group constant preprocessing is essential, since the degree of the correspondence of the resultant computational characteristics of the physical model of the system is largely dependent on correctness of the group partition choice. Evidently, the higher the number of the energy groups, the more accurate the computations, but the neutron transport computation time becomes longer with increasing number of the energy groups, with the dependence being more than linear, and the amount of required main memory increases. This issue will not be considered in this paper;

Selection of the spectral weight functions used in the computation of the group constants. The scheme would be an optimal option, in which neutron spectra of the relevant regions at different times of the system performance were used for the weight functions in the preprocessing of constants of different physical regions. Clear that the precise energy distribution of neutrons in different regions of the system is not known in advance (before the system computation). The neutron spectra obtained from computations of similar systems are used quite frequently in practice for the weight functions. In some cases some standard spectra (Maxwell spectra, fission spectra, etc.) are used for the weight functions.

A serious disadvantage of the above procedure of the group constant preprocessing is that the weight functions not corresponding to real energy distributions of neutrons in the computed systems are used. These deviations primarily affect the elastic scattering matrix as well as the results of reaction cross section averaging (for threshold reactions and reactions, whose cross sections depend crucially on energy). A possible method for reduction of errors due to inexact knowledge of neutron spectrum form is to increase the number of the neutron groups. This approach, however, has demerits considered above.

Another approach to resolution of this problem can be the one being developed by VNIIIEF. The idea of the approach is that during the problem computation the group constants are re-processed at each timestep, at which the neutron spectrum has changed significantly in any physical region of the system. The group constants are re-calculated using the neutron spectra corresponding to a given system state and multi-group sets of constants (several hundreds of groups) that have been created specially for this. In this approach, when using a relatively small number (a few tens) of groups, the results are comparable in accuracy to those of the computations on a significantly larger number (hundreds) of groups. The computational resources are therewith saved significantly, which is particularly important in solution of multidimensional problems. We called this approach: “dynamics re-calculation of constants”. The developing of this approach was the initiative of dr. Shagaliev.

Below is the schematic of the constant re-calculation approach (see Fig. 4)
As seen from the figure, the time-dependent neutron transport problem solution is divided into a number of looped steps:

1. Solve the neutron transport problem at timestep using a small number (on the order of several tens) of groups;
2. Analyze the need for the recalculation of the constants;
3. Construct the continuous spectral neutron distribution in each region from the data of the group computation;
4. Re-calculate the group constants for all isotopes of the problem using the multi-group system data and known continuous weight function;
5. Transfer to step (1) of the algorithm for the transport equation solution at the new timestep.

Note that step 3, i.e. development of the technique for the construction of the continuous energy dependency from the group neutron distributions, was the most complicated for the developers. At least, the following conditions should be met in this technique:

- The function to be constructed should be nonnegative and smooth enough.
- The function to be constructed should keep the integral numbers of neutrons unchanged in each group.
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• The construction algorithm should be reliable and inexpensive, as it is integrated into the general chain of the computations of nonstationary processes.

For the calculation of the smooth enough and, at the same time, non-negative spectral function approximating the array of group data, i.e. region- (material-) average values for the scalar field or neutron amount, several methods have been studied numerically. The most appropriate was the algorithm based on the solution to the problem of search for conditional minimum. The idea of the method is the following.

There is array \( u_i \ (i = 0, 1, \ldots, n) \) that gives a partition into groups. The authors of the technique chose lethargy \( u_i = \ln \frac{10}{E_i} \), where \( E \) is energy in MeV. For each group \( i \) \((u \in [u_{i-1}, u_i])\) there is array \([f_i \Delta u_i]\) \((\Delta u_i = u_i - u_{i-1})\) obtained from the few-group computation. It has been detected that it is best to use for the array \([f_i \Delta u_i]\) the quantity that gives the number of neutrons in the region.

The desired spectrum \( f(u) \) is approximated by the set of continuous functions \( f_i(u) \) given on the associated intervals \([u_{i-1}, u_i]\). The following conditions are imposed on the functions \( f_i(u) \):

- \( f_i(u_i) = f_{i+1}(u_i) \);
- \( \int_{u_{i-1}}^{u_i} f_i \, du = \bar{f}_i \Delta u_i \).

At edges zero conditions are given: \( f_i(u_0) = f_n(u_n) = 0 \). Polynomials of a degree no higher than 3 have been used for \( f_i(u) \).

As the objective function we define function

\[
Y(z_1, z_2, \ldots, z_{n-1}) = 0.5 \sum_{i=2}^{n} y_i^2 ,
\]

where

\[
z_i = f_i(u_i), \quad i = 1, 2, \ldots, n - 1;
\]

\[
y_i = \omega_i (f_{i-1}'(u_{i-1}) - f_i'(u_{i-1})), \quad i = 2, \ldots, n.
\]

The \( f_{i-1}'(u_{i-1}) - f_i'(u_{i-1}) \) determines a discontinuity in the derivative approximating the functions at the group bounds, and weight vector \( \omega \) is needed to give the "value" of one or another discontinuity in the objective function calculation, the larger is the \( |\bar{f}_{i-1} - \bar{f}_i| \), the closer to zero is the \( \omega_i \). The need for setting the weights stems from the experience gained in the computations. Initially the computations were conducted with the objective function without weights \( (\omega_i \equiv 1) \), and it has been found that the method attempts to
equalize derivatives of parabolas primarily at the boundaries with large differences in the values of $\ddot{F}$. On the other hand, it is best to smooth the function, where there are no large gradients, while at the group bounds with large differences in average values we can restrict ourselves to not very smooth approximation. A good choice can be formula

$$\omega_i = \frac{\min (\ddot{f}_{i-1}, \ddot{f}_i)}{\max (\ddot{f}_{i-1}, \ddot{f}_i)} \times \frac{\min (\Delta u_{i-1}, \Delta u_i)}{\max (\Delta u_{i-1}, \Delta u_i)}.$$

The task is to find the objective function minimum with account for limitations like

$$0 \leq z_i \leq C_i, \quad i = 1, 2, ..., n - 1,$$

which guarantee nonnegativity of the polynomials $f_i(u)$ on the relevant intervals of $u$. For example, when using the piecewise-parabolic approximation, $C_i = \min (3\ddot{f}_{i-1}, 3\ddot{f}_i)$ can be given. More complex (and more accurate) limitations have been studied, but they were abandoned in favor of the algorithm speed and reliability.

To resolve the problem of search for the minimum with simple (constant) limitations, the Newton method has been used. In so doing equation systems with tridiagonal matrix (for the case of the piecewise-parabolic approximation) are solved with the factorization method in iterative loop.

The technique and algorithm for the re-calculation of the group constants from the multi-group ones using the continuous function $f(u)$ obtained at the previous step (step 3) of the computation for the new weight function are standard, so we need not go into their details here.

To demonstrate the above described algorithm efficiency, we present below the results of calculations of parameter $K_{\text{eff}}$ for critical assembly hmf933 (Table 1) from BEAR archive. Table 2 gives deviations (in percentage terms) from the experimentally obtained values of $K_{\text{eff}}$ for computations with 14- and 26-group partition with and without dynamic recalculations of constants. Six (6) recalculation iterations were used in computations with dynamic recalculation, i.e. the values of constants were specified 6 times using the neutron spectrum from the previous iteration.

**Table 1. Hmf933 critical assembly composition.**

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<th>Density, g/cm³</th>
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<th>Concentration, nuclei/barn/cm</th>
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<td></td>
<td>Ni</td>
<td>4.2854e-4</td>
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</table>
### Table 2. Departure (%) $K_{\text{eff}}$ from experimental result.

<table>
<thead>
<tr>
<th>Number of groups</th>
<th>Without re-calculation</th>
<th>With re-calculation</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Departure $K_{\text{eff}}$ (%)</td>
<td>Iterations Number</td>
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<tr>
<td>14</td>
<td>1.49</td>
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<tr>
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<tr>
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### Conclusion

The paper discusses the system of constant support of neutron-physical computations that has been developed by VNIIEF, approaches to and methods for data manipulations, which are aimed at a higher accuracy and reliability (i.e. correspondence to the class of physical problems being solved) of the group constants used in solution of neutron transport problems. The paper particularly describes:

- Approaches to assessment of the “quality” of evaluated spectral constants and development of recommendations on their use for solution of one or another physical problem;
- The technique for refinement of the group constants during the neutron transport problem solution. The idea of the technique is that during the problem computation the group constants are re-processed at each timestep, at which the neutron spectrum has changed significantly in any physical region of the system. The error due to inaccurate neutron spectrum form in the group constant preprocessing becomes thereby reduced.

### References


R. E. MacFarlane and D. W. Muir


