Institute of Theoretical and Mathematical Physics

Russian Federal Nuclear Center -

VNIIEF

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

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Abstract

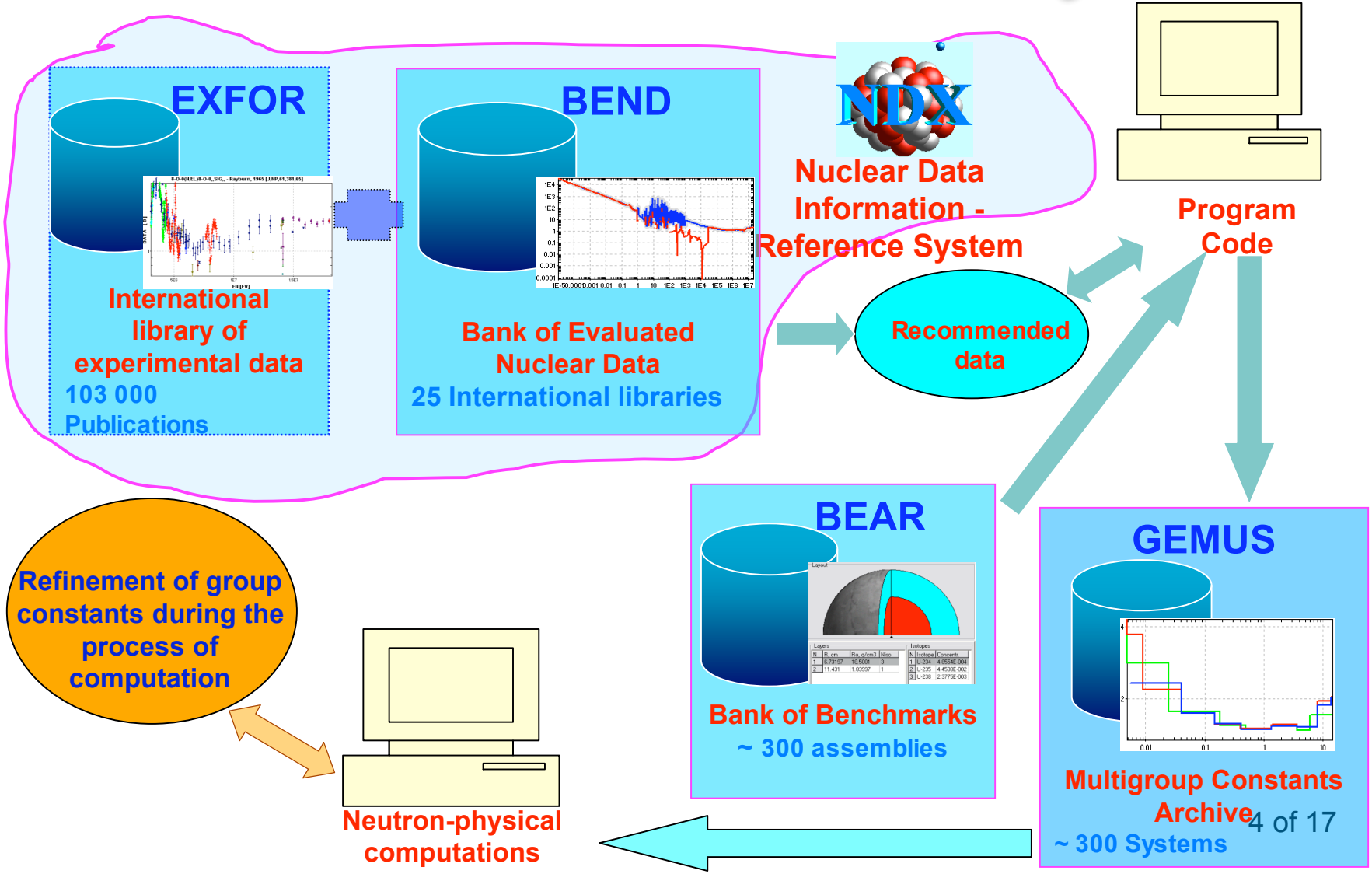
The paper discusses the system of constant support of neutron-physical computations that has been developed by VNIIEF. The principal task, which to tackle the system has been just developed for, above all is a higher “quality” of the preprocessing of group macroscopic neutron constants and constants of γ-generation and γ-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.

"Quality" of the Group Neutron Constants

The Factors:

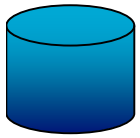
- Correspondence of the source spectral data used for the group constant preprocessing to a specific problem to be solved or problem class ;
- Correctness of the choice of the group energy partition for the problem;
- The group constant preprocessing method, which is determined by specific computational algorithms and proper choice of weight functions (which are typically unknown in advance) used in the computations;

General Scheme of Constant System



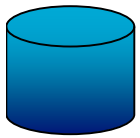
Main Components - Databases

Bank of Evaluated Nuclear Data BEND



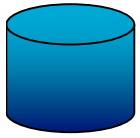
25 International and Recommended Libraries, 9000 Isotopies,1.5 Gbytes ENDF/B-6, JENDL-3.3, JEF-3, CENDL-2, BROND-2 …. ;

International Experimental Data EXFOR



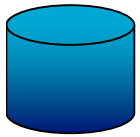
103 000 publications, 0.5 Gbytes; cross-section, Integral Measurements, Differential Data;

Bank of Benchmarks BEAR



~ 300 spherical and cylindrical systems ;

Archive of Multigroup Constants GEMUS



~300 Systems for Various Purposes;

Main Components - Code

Program Code BEND:

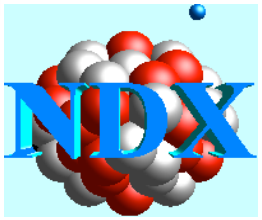
- Pointwise cross-sections reconstruction from resonance parameters;
- Doppler broadening cross section calculation for different temperatures of medium;
- Calculation of effective spectral values accounting chemical bonds of atoms;
- Calculation of self-shielded multigroup neutron data and photon production.

Program Library MARX

- Calculation of macroscopic group constants for neutron-physical computation;
- Refinement of group constants during the process of computation.

Main Components - Shell

Nuclear Data Information - Reference System



Component of the computer automated workstation of the specialist in the area of nuclear-physical data.

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

NDX - Databases

- 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;
- Data from the table of nuclear masses and reaction energies by Audi and Wapstra;
- Data from the International Base ENSDF on atomic nucleus structure, 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;
- Data of prompt fission products. Chains of radioactive decays of fission products.

NDX - Capabilities

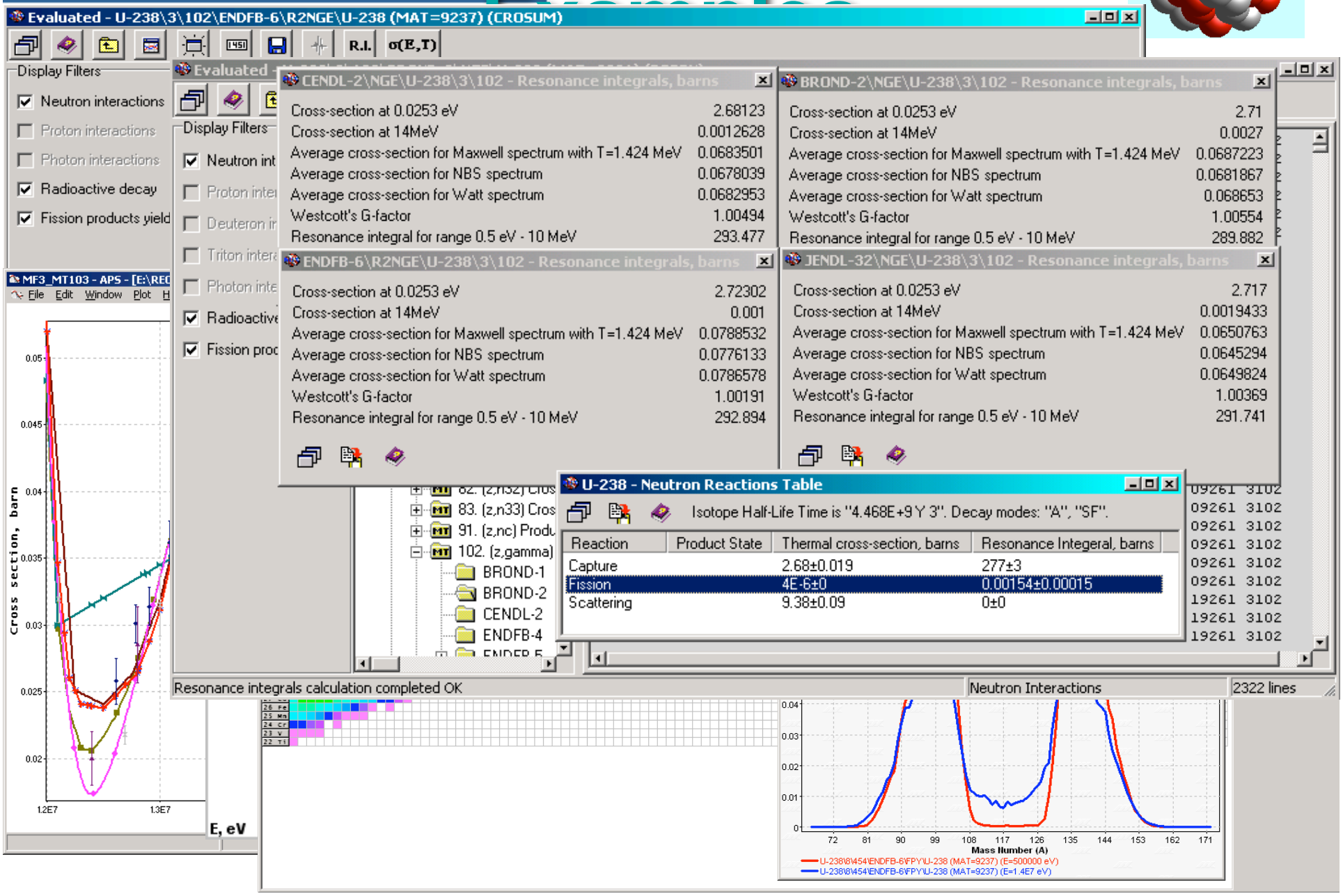
- Tabular scanning and construction of 2D and 3D graphs of different quantities, with the possibility to superimpose the dependencies on one graph for their comparison and comparison of them to the experimental data of the EXFOR library ;

- 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.

5-I.C, 19-23 June 2005, Vienna Austria

Example



(Factor # 1)

"Quality" of Evaluated Spectral Constants

Main Approaches:

- 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;
- Comparison of calculated integral characteristics (average cross sections in different characteristic spectra, resonance integrals, Westcott's G-factors, etc.) to experimental or recommended data;
- Calculations of parameters of benchmarks simulating a certain problem class.

Goal:

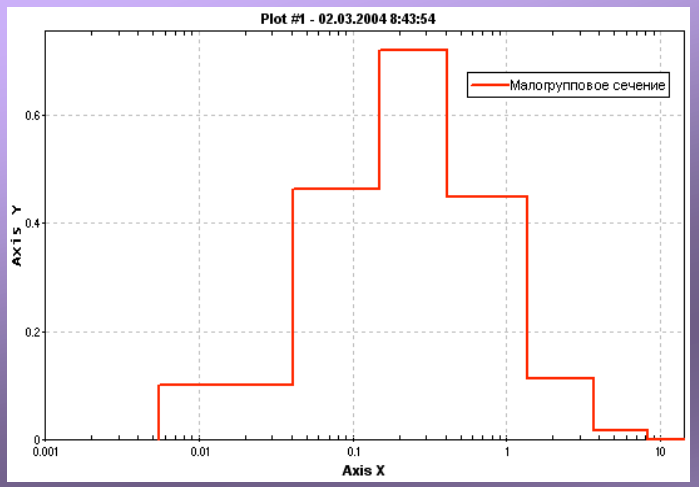
Library of Recommended Constants

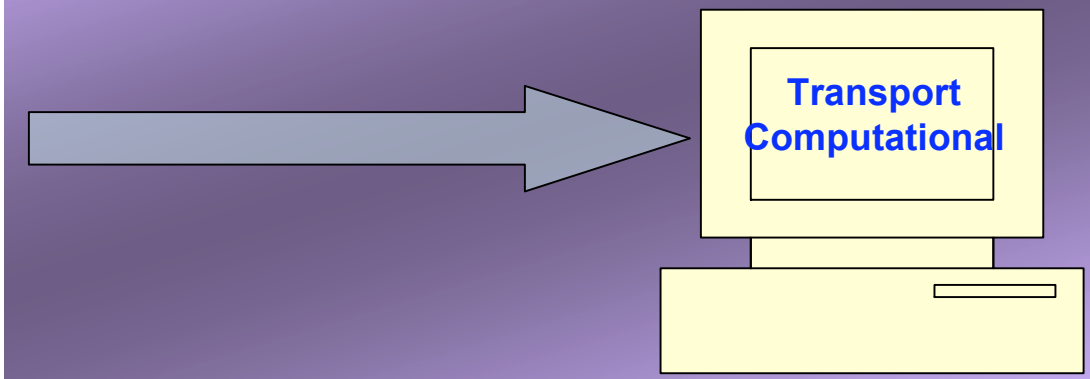
(Factor # 3)

"Undefined Weight Function"

Standard Approach:

- Assessment of applicability of neutron-physical characteristics of isotopes from different libraries of evaluated data for calculation of a certain problem class;
- Selection of the group energy partition;
- Selection of the spectral weight functions (undefined) used in the computation of the group constants. Calculation of group constants system.





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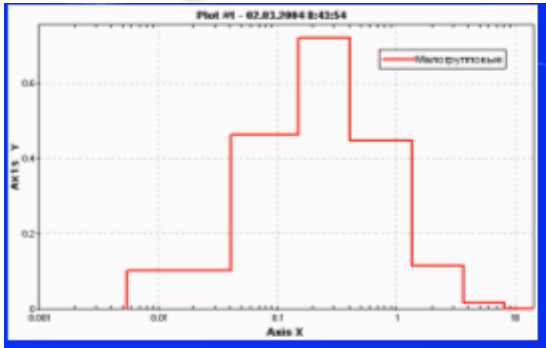
(Factor # 3)

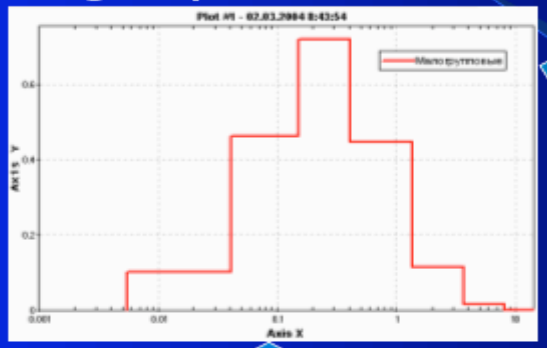
"Dynamics re-calculation of Constants"



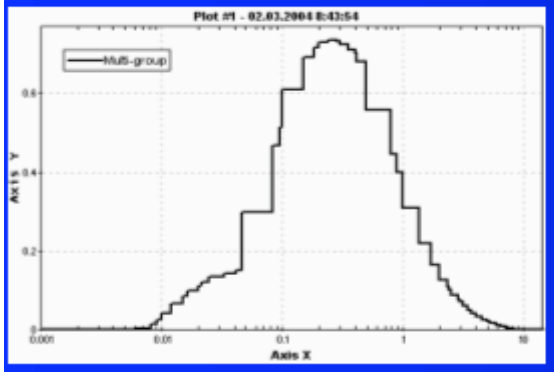
Initial group constants

TRANSPORT COMPUTATION

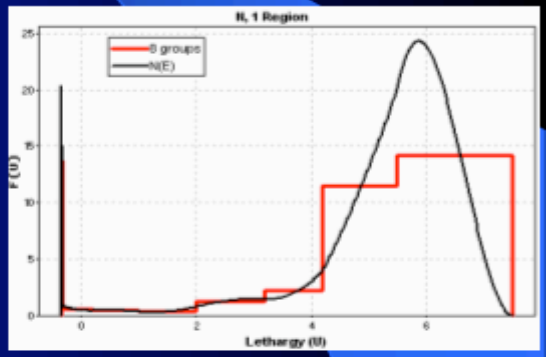
Re-calculated group constants



Criterion of the re-calculation



Multi-group constants



Construction of the neutron function

Re-calculation of the group constants

(Factor # 3)

Reconstructions Algorithm

$$u_i\,(i=0,1,\ldots,n)\,,\quad u_i=\ln 10/E_i\,,\quad u\in[u_{i-1},u_i]\,,\quad \Delta u_i=u_i-u_{i-1}$$

Let:

$$f_i(u)=a_i(u-u_i)^2+b_i(u-u_i)+c_i;$$

OR

$$f_i(u)=a_i(u-u_i)^3+b_i(u-u_i)^2+c_i(u-u_i)+d_i;$$

$$f_i(u_i)=f_{i+1}(u_i)$$

$$\int_{u_{i-1}}^{u_i} f_i\,du=\bar{f}_i\Delta u_i$$

$$f_1(u_0)=f_n(u_n)=0$$

Objective Function:

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

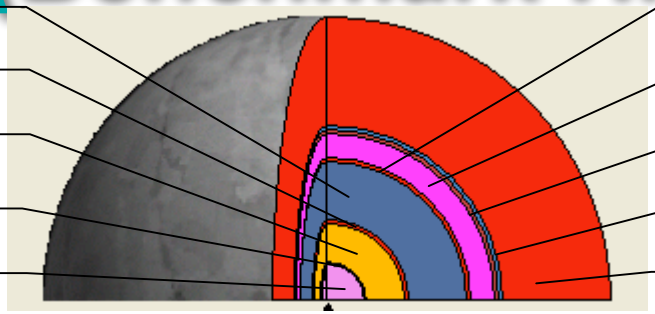
Where

$$z_i=f_i(u_i),\qquad i=1,2,\ldots,n-1;$$

$$y_i=\omega_i\left(f'_{i-1}(u_{i-1})-f_i'(u_{i-1})\right),\quad 0\le z_i\le C_i,\qquad i=1,2,\ldots,n-1$$

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

(Factor # 3) Test (Benchmark Hmf933)



Number of groups	Without re -calculation	With re -calculation	
	Departure Δ_{eff} (%)	Iterations Number	Departure Δ_{eff} (%)
14	1.49	1	1.19
		2	0.23
		3	0.17
		4	0.11
		5	0.09
		6	0.09
26	0.73	1	0.19
		2	0.04
		3	0.02
		4	0.02
		5	0.01
		6	0.01

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.

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