

# Probabilistic Representation of Resonance Structure in Nuclear Safety Applications

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## Introduction

The probability tables are included in the top level hierarchy [1] as the reconstructed cross section element, connected with the unresolved resonance region. It looks like as a restriction for applications, which use extended or generalized modifications of this representation. In particular, some nuclear safety studies need in approaches, which decrease time consumption due to effective representation of resonance structure. As an example, two data libraries are considered:

- group cross-sections and self-shielding factors data libraries for analyses of hypothetical incidents with reactor core destruction, prepared by the C4R+C4P code system [2,3] for SIMMER code [4], assigned to safety analyses of advance reactor concepts;
- group cross section data library with generalized subgroup parameters, for criticality calculations of extended and loosely coupled systems with high heterogeneity ( the spent fuel pools, for example) by the SAPFIR code package [5].

The extended forms of probability tables are described, to discuss possibility to place them in the hierarchy of the GND structures.

## 1. Probabilistic representation

$P(\sigma)$  description of neutron cross sections with resonance structure, proposed in [6],[7], has found continuation and extension in numerous studies. Large variety of algorithms, dedicated to parameterization and applications these data in different neutron physics calculations, has been developed [8 - 18]. Two of them, implemented in the GRUCON package, are described in this paper.

According this approach, any cross section  $\sigma(E)$  in some energy interval  $\Delta E$  or "group" ( in some cases group can degenerate to energy point) can be described by probability distribution function

$$P(\sigma) = \sum_i \left| \frac{dE_i}{d\sigma} \right|$$

The cross section  $\sigma(E)$  can be characterized by interaction type (r), temperature (T), target nuclide (ZA), or, for brevity, by "x". For any pair of cross section distributions,  $P(\sigma_x)$  and  $P(\sigma_y)$ , defined in the same group, can be calculated so called "conditional" distribution function  $P(\sigma_y / \sigma_x)$ , defined as distribution of  $\sigma_y$  under fix value of  $\sigma_x$ .

In common use, the probability distribution functions are approximated by series:

$$P(\sigma_x) \sim \sum_{i=1}^{N_x} a_i^{(x)} \delta(\sigma_x - \sigma_i^{(x)}),$$

$$P(\sigma_y | \sigma_x) \sim \sum_{j=1}^{N_y} \sum_{i=1}^{N_x} \omega_{j,i}^{(y,x)} a_i^{(x)} \delta(\sigma_x - \sigma_i^{(x)})$$

Where:  $a_i^{(x)}, \sigma_i^{(x)}, \omega_{j,i}^{(y,x)}$  is a set of parameters (usually named, as weights, cross sections and correlation coefficients, correspondingly), with physical constraints:

$$\sum_{i=1}^{N_x} a_i^{(x)} = 1, \quad a_i^{(x)} > 0,$$

$$\sigma_{\min}^{(x)} \leq \sigma_i^{(x)} \leq \sigma_{\max}^{(x)},$$

$$\sum_{j=1}^{N_y} \sum_{i=1}^{N_x} \omega_{j,i}^{(y,x)} = 1, \quad \omega_{j,i}^{(y,x)} \geq 0,$$

$\sigma_{\min}^{(x)}, \sigma_{\max}^{(x)}$  - minimal and maximal values of  $\sigma_x(E)$  in the group.

Different subsets of "subgroup" or "multiband" parameters, or "probability tables", with specific constraints and relations, will be referred lower, for generality, as "probabilistic representation".

## 2. Computing algorithms

Among numerous algorithms and calculation schemes, developed for generation of specific set of probabilistic representation parameters, it is possible to distinguish two main approaches:

**Approach 1.** The parameters are defined from a system of nonlinear equations, binding group averaged parametric functions and subgroup weight and cross sections, with consequent optimization procedure, to minimize approximation error for required functional (self-shielding factors and Doppler increments, for example). Two types of equation systems (or similar them) are usually employed in this approach:

$$(a) \langle (\sigma_x + S_0)^{n-L} \rangle = \sum_{i=1}^N a_i^{(x)} (\sigma_i^{(x)} + S_0)^{n-L}, \quad (\text{Gauss, or Pade-I technique [9]}), \text{ or}$$

$$(b) \langle 1/(\sigma_x + S_n) \rangle = \sum_{i=1}^N a_i^{(x)} / (\sigma_i^{(x)} + S_n), \quad (\text{Pade-II [13], Pade-IIm [15] techniques})$$

Where

$\langle \dots \rangle$  - averaging procedure in energy interval or energy point (in case of statistical description of unresolved resonance structure);

$n=1, 2, \dots, 2*N$ ;

$N, L, S_0, \{S_n\}$  - required or assigned function parameter values.

Each of this equation system has unique solution for specific "x" value, which can be used as "zero" approximation for construction and search some consistent set of parameter values in required "x" subspace.

**Approach 2.** Numerical integration of detailed cross-section, as function of energy, in required or assigned (after preliminary study of cross section behavior) cross section bands  $[\sigma_i, \sigma_{i+1}]$ . The energy positions of each cross section band can be used in calculation of correlation matrices.

There are also calculation schemes, in which these two approaches are combined - so-called "Synthetic Approach".

### 3. Probabilistic data processing

#### 3.1 The GRUCON standard structures and modules

The approaches, mentioned above, are implemented in the GRUCON functional modules. To keep probabilistic representation parameters, three GRUCON standard structures are used:

- \*P\* - subgroup weights and cross sections,
- \*PN\* - subgroup numbers, ordered in energy  $N(E)$ ;
- \*PC\* - correlation matrices.

The \*P\* structure allows to keep several parameter sets, with different constraints and relations, depending on destination. In particular, subgroup weight can have single value for all temperature and reactions, or list of values for temperatures, or table of values for temperatures and reactions, depending on their destination and calculation technique. Two approaches to subgroup generation task have been implemented in frame of GRUCON package:

The GRUCON functional content, designed to probabilistic data processing, includes

- processing modules:
  - F/E-P - calculate subgroup parameters from the moments by Approach 1;
  - S/-P-PN - calculate of subgroup parameters from cross-section tables by Approach 2;
  - PN/PN-PC - calculate subgroup correlations matrices for reactions, temperatures, isotopes;
  - PN/EA-PC - calculate subgroup correlation matrices for collisions;
  - PN/P-S - prepare subgroup cross-sections, as function of energy;
  - P/D-F - calculate cross section functions from subgroup parameters;
  - P/PC-P - collapse subgroups parameters with correlation matrix, to get average value for temperature or reaction;
  - P/P-P - "glue" two subgroup tables together,
- converters:
  - BNAB - write to the BNAB group data library
  - TEMBR - write to the TEMBR group data library
  - ACE - write to ACE files
  - PENDF - read from PENDF files.

Different forms of probabilistic representation are demonstrated on the Figs.1-6.

In Fig.1, self-shielding f-factors for U238 and U235, calculated from point-wise cross-sections (the S/G-F module), and approximated by subgroup parameters (the F/E-P + P/D-F modules), are presented.

In Fig.2, the resonance cross sections of U238 - on the left side, and U235 - on the right side, in detailed (lines) and subgroup (NSUB=30, stairs) representations are compared in energy group  $\Delta E=4.65-10\text{eV}$  (NG=6);

In Fig.3 the total cross sections are presented in form of probability density functions, obtained with NSUB=30 (points) and NSUB=300 (lines) subgroup numbers.

The subgroup correlation matrices for U-238 in the energy interval  $\Delta E=4.65-10\text{eV}$  (NG=6) for NSUB=30, are shown:

in Fig.4 - total cross section correlations for temperatures  $T=300\text{K}$  and  $T=2100\text{K}$ ,

in Fig.5 - total cross section correlations in collisions for  $T=300\text{K}$ ,

in Fig.6 - the U238 and U235 total cross sections correlations,  $T=300\text{K}$ .

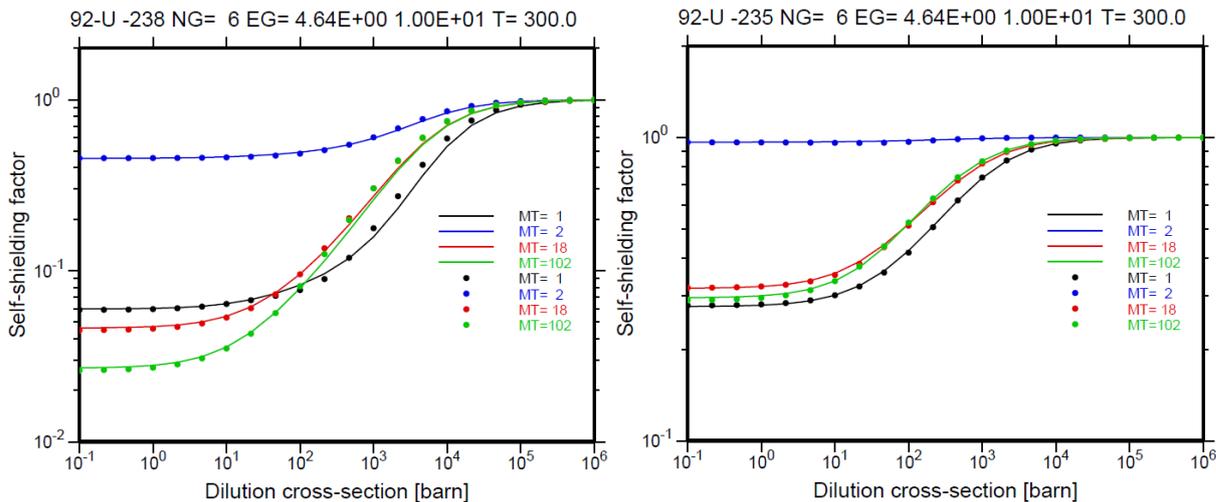


Fig.1 U-238 (left) and U-235 (right) self-shielding factors, obtained through the S/G-F ( lines) and F/E-P + P/D-F modules, for NSUB=4 (points), in energy group  $\Delta E=4.65-10$  eV

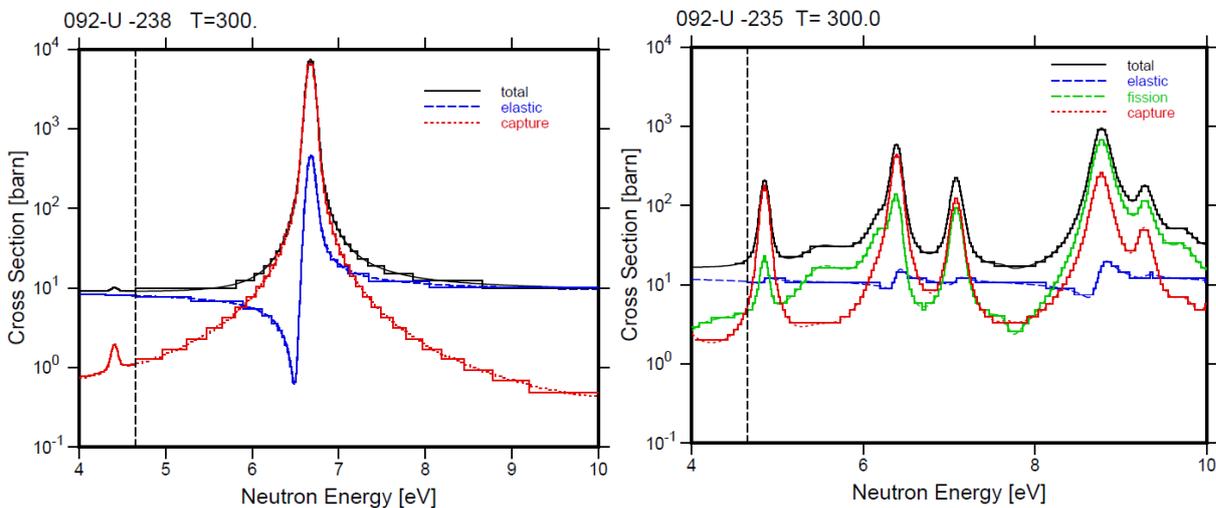


Fig. 2 The U238 ( left) and U-235 (right) cross sections in point-wise and subgroup stairs forms

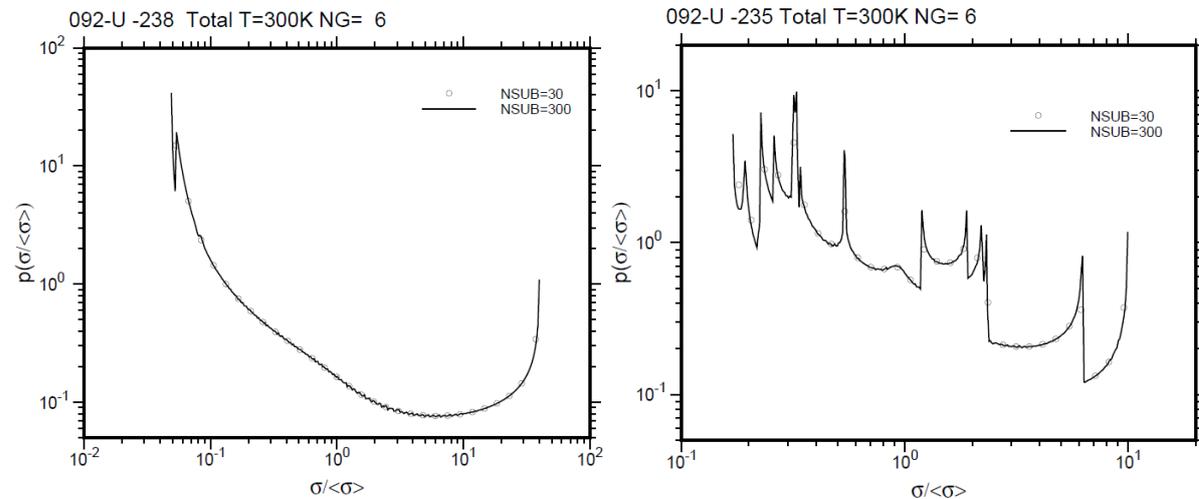


Fig. 3 The U238 (left) and U235 (right) total cross-section probability density functions

092-U -238 NG= 6  
 ls1=ls2= 1 T1= 300.0 T2=2100.0

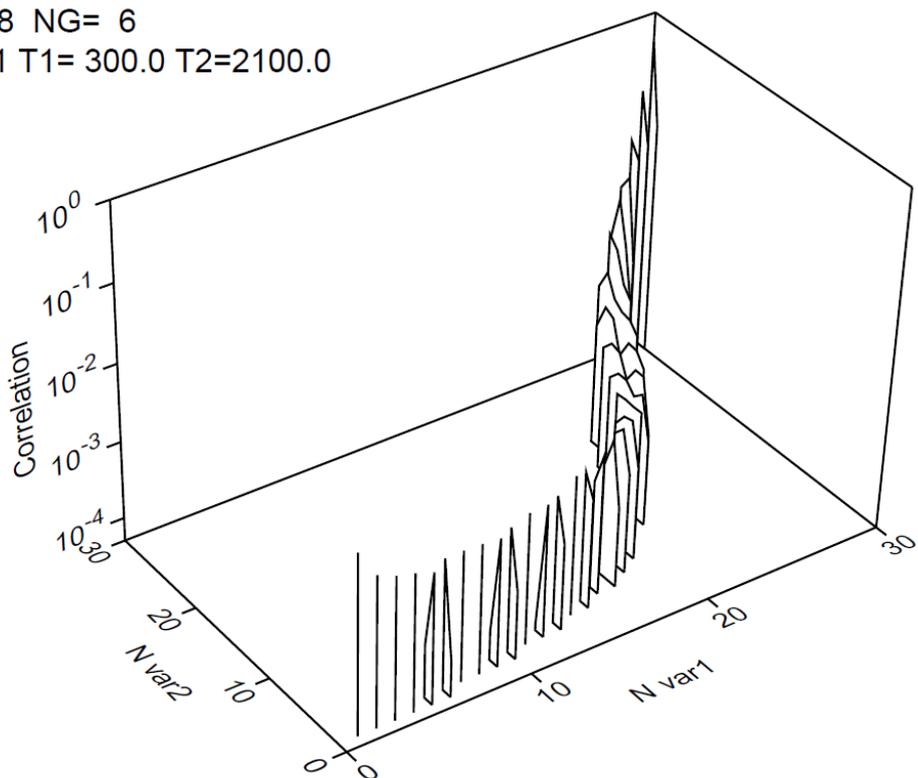


Fig.4 Correlations in the U238 total cross sections at T=300K and T=2100K

092-U -238 NG= 6  
 ls1= 1 ls2= 1 T1= 300.0 T2= 300.0

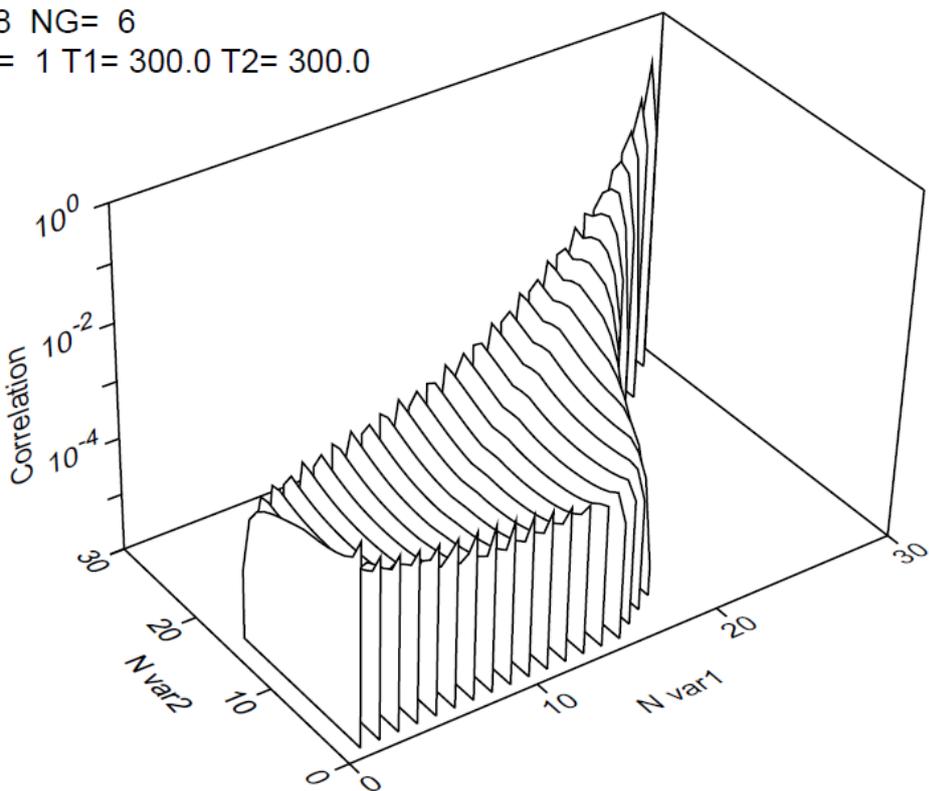


Fig.5 Correlations in the U238 total cross-sections at neutron collisions

092-U -238 092-U -235 NG= 6  
 ls1=ls2= 1 T1,T2= 300.0

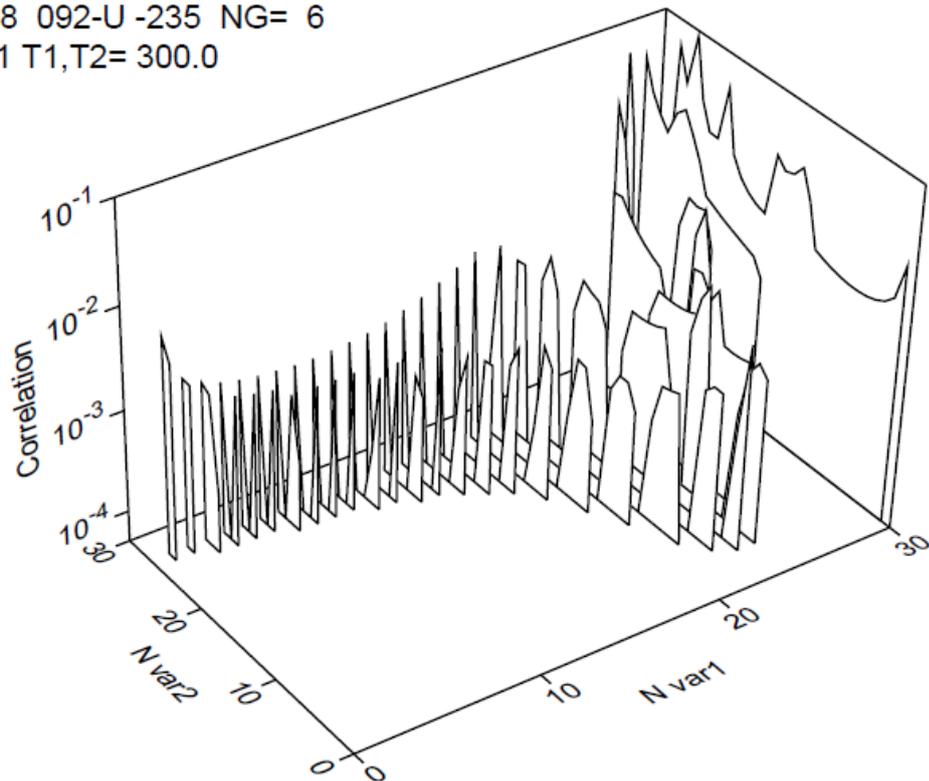


Fig.6 The  $U^{238}$  and  $U^{235}$  total cross section correlations

### 3.2 C4R+C4P processing system

The C4R+C4P processing system has been developed in the IKET/KIT (Karlsruhe) to generate problem-oriented cross-section libraries for SIMMER safety code. The C4P code package supports group data in the CCCC (ISOTXS+BRKOXS) extended format, which includes thermal scattering data. Data in this format can be obtained from the GENDF files by C4R converter (an analogue of the CCCCR module of NJOY[19]).

The C4P code package consists of modules:

- BINX - converts CCCC data from binary to ASCII and back,
- LUNX - splits each isotope in a separate file and,
- LINX - joins CCCC data files (all isotopes in 1 file),
- CONX - reduce number of groups using user-supplied spectra,
- MINX - makes mixtures of isotopes ( or “convolution procedure”, see below),  
by employing the “extended probability tables” ,
- SUBX - calculates subgroup parameters,
- GOXS - converts to the GOXS (MACRXS) format

### 3.3 Convolution procedure and extended probability tables

To prepare self-shielding factors ("f-factors") for isotope mixtures, convolution procedure is used.

F-factors can be calculated as follows:

$$F_r(T, \sigma_0) = \frac{M_r(\sigma_0)}{M(\sigma_0)},$$

$$M(\sigma_0) = \sum_{\bar{i}} a_{\bar{i}} \frac{1}{\left( \sum_c \rho_c \sigma_{i(c)} + \sigma_0 \right)},$$

$$M_r(\sigma_0) = \sum_{\bar{i}} a_{\bar{i}} \sum_c \frac{a_{i(c)}^{(x)}}{a_{i(c)} (\rho_c \sigma_{i(c)}^{(t,x)} + \sum_{c' \neq c} \rho_{c'} \sigma_{i(c')} + \sigma_0)}$$

where:

$$a_{\bar{i}} \equiv \prod_{c=1}^{NC} a_{i(c)},$$

$$\sum_{\bar{i}} \{ \dots \} \equiv \sum_{i(1)=1}^{I(1)} \sum_{i(2)=1}^{I(2)} \dots \sum_{i(NC)=1}^{I(NC)} \{ \dots \}$$

$\rho_c$  - nuclear density of c-isotope.

To find required set of parameters, *Padé-II* technique with optimization procedure ( by selection the set of  $\sigma_0$ , minimizing the approximation error), is employed:

$$\langle 1/(\sigma + \sigma_0) \rangle \approx \sum_{i=1}^N a_i / (\sigma_i + \sigma_0),$$

$$\langle \sigma_x / (\sigma + \sigma_0) \rangle / \langle \sigma_x \rangle \approx \sum_{i=1}^N a_i^{(x)} / (\sigma_i^{(x)} + \sigma_0)$$

The "extended" probability table technique assumes, that "total" subgroup cross-sections are always considered in combination with a certain "partial" subgroup cross-section; therefore several sets (instead of unique set) of the " total" subgroup values - for the total and for a few partial cross-sections - are computed. Consequently, the generation of the extended probability tables is significantly facilitated. The accuracy is improved since each f-factor table can be approximated independently from others (related to another cross-section type).

The algorithm of collapsing procedure is realized in the F/C-F module of GRUCON and the MINX module of C4P code systems.

#### 4. Purposes and Requirements

(A) Historically, the first consumer and distributor of the probabilistic data was the BNAB (or ABBN) [20] group cross section library for fast reactor and radiation shielding studies. This library includes balanced set of subgroup parameters, consistent with self-shielding factors. BNAB library contains:

$a_i$  - subgroup weights ( independent on reaction type and temperature),

$\sigma_i$  - total cross sections and

$\sigma_i^{(x)}$  - partial cross sections ( with temperature interpolation),

with balance constraints:

$$\sum_{i=1}^N a_i \sigma_i^{(x)} = \langle \sigma_x \rangle, \quad \sum_x \sigma_i^{(x)} = \sigma_i$$

(B) SIMMER code family [4] is developed and applied by JNC(Japan), KIT(Germany), CEA and IRSN(France), NEA(Italy) and other partners, for safety studies of nuclear reactors.

It includes a neutronics (coupled with thermal-hydraulics and structure) model that employs (for neutron flux and reactivity calculations) multigroup composition-dependent cross-sections. They are computed for each reactor node at each shape/reativity step during a transient simulation, the fluid-dynamics model of the code providing mesh-wise temperatures and densities for the fertile and fissile fuel components, structure, coolant, and control materials, their isotopic composition being constant during the transient. It allows to prepare compositions in advance, by convolution procedure, described above. The set of parameters needed, is:

$a_i, a_i^{(x)}$  - total and partial subgroup weights,

$\sigma_i, \sigma_i^{(x)}$  - total and "conditional" subgroup cross sections.

(C) SAPFIR-2006 [5] is a package of code and data libraries, developed in the "Kurchatov Institute" with the aim to extend scope of the Monte Carlo method to cover the VVER nuclear criticality safety applications, including substantiation of nuclear criticality safety, handling of nuclear fuel on the NPP with VVER, modeling severe accident with core disruption and fuel fusion. The SAPFIR data library contains 26-group cross section with "generalized" subgroup parameters, similar to the BNAB system (A), but supplemented by correlations matrices:

$a_i$  - subgroup weights,

$\sigma_i$  - subgroup total cross sections,

$\sigma_i^{(x)}$  - subgroup partial cross sections;

$\omega_{j,i}^{(T',T)}$  - correlation matrix for total cross sections with  $T$  and  $T'$  temperatures,

$\omega_{j,i}^{(ZA',ZA)}$  - correlation matrix for total cross sections of  $ZA'$  and  $ZA$  isotope,

$\omega_{j,i}^{(NC+1,NC)}$  - correlation matrix for total cross sections in sequence of collisions

The parameters generation procedure is based on synthetic approach, in which analytical solution (Approach 1a) is used to define optimal bands for numerical integration of detailed cross sections ( Approach 2).

## 5. Benchmarking

The validity and effectiveness of probabilistic representation has been tested in integral calculations, performed by the MCNP and DANTSYS code systems for point-wise and group-wise working data libraries, prepared through GRUCON and NJOY+C4R+C4P processing codes in the ACE and CCCC (ISOTXS and BRKOXS) data formats.

### 5.1 Performance of convolution procedure

560-group data library (a subset of 1968-group set developed for the ERANOS code system) has been prepared in the CCCC extended (for taking properly into account thermal scattering data for neutrons and include subgroup parameters) format.

The ENDF/B-VI.8, JEF-2.2, JEFF-3.0, JENDL-3.3 evaluated data libraries were processed in detailed (ACE) and group-wise (GENDF) forms by using a standard weighting function (fission spectrum at higher energies; Fermi spectrum,  $1/E$ , in resonance energy region; Maxwellian spectrum at thermal energies) into a master library for 9 temperatures (from 300K to 6000K), 16 dilution cross section (for f-factors) and 6 angular moments. The GENDF data were converted to the CCCC master files and CCCC master library was formed by the C4R+C4P code system. Extended probability tables were obtained with tolerance parameter value 0.1%.

Characteristics of extended probability parameters are shown in Figures below:

in Fig.7 (left) - approximation errors in moments and f-factor for U238 in each energy group,

in Fig.7 (right) - approximation errors in moments and f-factor all materials,

in Fig.8 (left) - maximal number of subgroup for Fe-56, U-238 and Pu-239 nuclides in each energy group,

in Fig.8 (right) - maximal number of subgroups for all group and all nuclides.

Nuclide is identified by flag  $ZA=Z+0.001*A$ .

With this master library, nine homogeneous models related to reactors, which can be potentially used for burning Pu and minors actinides (MAs), were studied:

1. **ADS-DED** -Dedicated (Pu and MAs) nitride fuel, Pb coolant,
2. **ADS-ThU** - Th/U-233 fuel, Pb coolant,
3. **ADS-XADS** - MOX fuel, Pb coolant,
4. **ADS-XADS-Bi** - MOX fuel, LBE coolant,
5. **EFR1** - MOX fuel, Na coolant,
6. **MOLT** - Molten salt (FLIBE) with U-235/U-238, graphite moderator,
7. **MOLT-U3** - Molten salt (FLIBE) with Th-232/U-233, graphite moderator.
8. **SCFBR1** - MOX fuel, supercritical water (fast option),
9. **SCFBR1-Cm** - MOX and MAs fuel, supercritical water (fast option)

Four states were considered for each model in order to investigate major reactivity effects: a cold state, at  $T=300K$ , (2) a hot state, at  $T=1200K$ , (3) the cold state without coolant or moderator, (4) the hot state without coolant or moderator. In Table I one may see the performance of the isotope-mixing procedures based on the extended subgroups technique. The first two columns of Table I show the MCNP  $k$ -inf values and corresponding ( $1\sigma$ ) uncertainties. The next two columns (ISOTOPES) show the  $k$ -inf values obtained with 560-group "isotope-wise" cross sections and the corresponding deviations from the MCNP results. The next two columns (ELEMENTS) show results of similar 560-group calculations with "element-wise" (natural mixtures and enriched fuel) data, prepared by collapsing procedure, with deviations from the ISOTOPE results. The number of "nuclides" is reduced (compare NISOT and NELEM parameter values). The last two columns shows "material-wise" results with deviations from ISOTOPE calculations, with three or four "nuclides" being used: fuel (one or two), structure, and coolant. The thermal-hydraulic part of SIMMER computes densities and temperatures of these "materials". Therefore, using of material-wise data saves computing time.

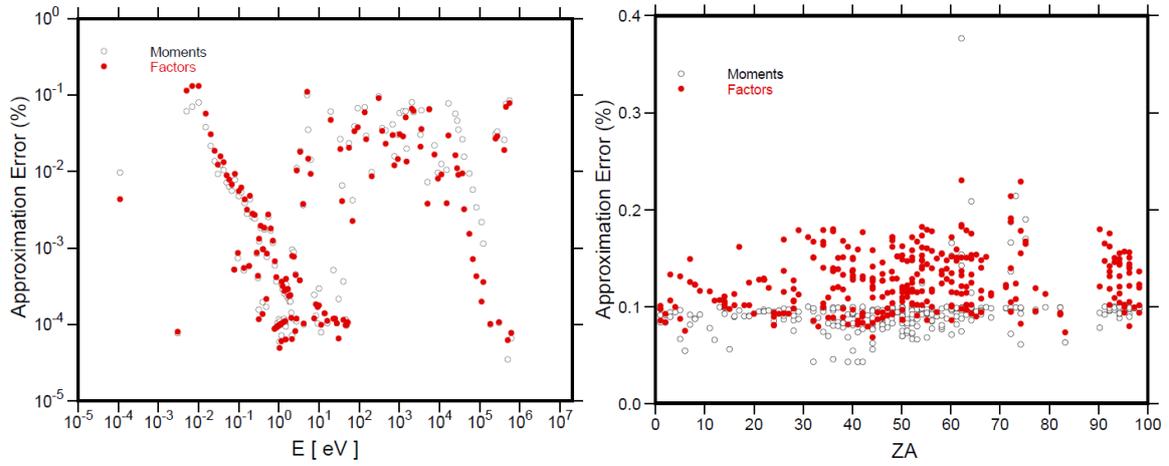


Fig.7 Approximation errors for U238 (left) and all nuclides (right) of the ENDF/B-VI.8

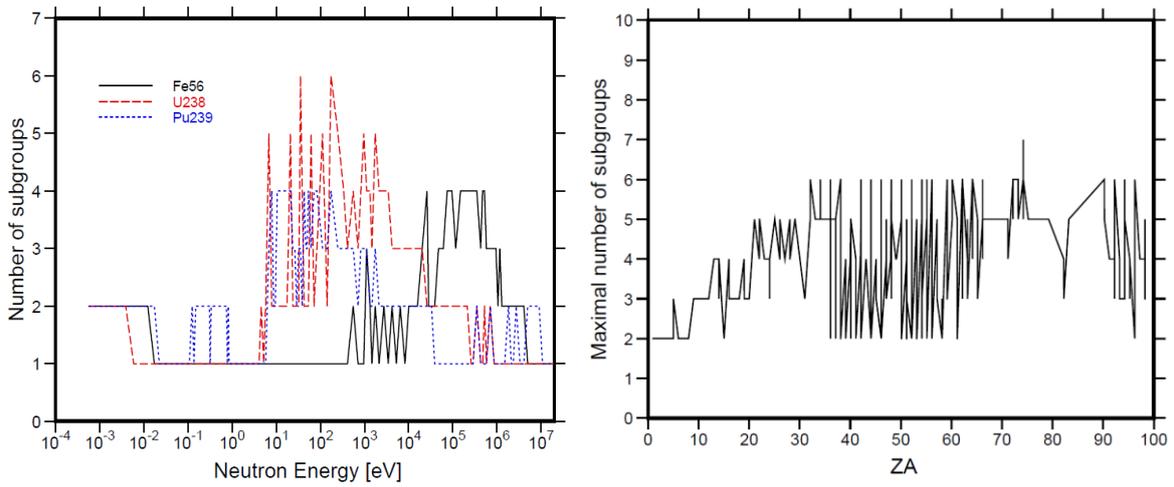


Fig. 8 Maximal numbers of subgroups in each group for the Fe56, U238 and Pu239 (left) and for all groups and for all nuclides (right) of the ENDF/B-VI.8

Table I. K-inf values with isotope wise, element-wise and material-wise data

Composition	State	MCNP	$\Delta K$	ISOTOPES	$\Delta IM$	ELEMENTS	$\Delta EI$	MATERIALS	$\Delta MI$
				<b>NISOT=31</b>		<b>NELEM=10</b>		<b>NMAT=4</b>	
ADS-DED	300	1.12669 $\pm 34$		1.12589	-63	1.12597	6	1.12596	5
	1200	1.12604 $\pm 32$		1.12524	-64	1.12531	6	1.12530	5
	300v	1.22353 $\pm 39$		1.22222	-89	1.22230	6	1.22228	5
	1200v	1.22268 $\pm 37$		1.22157	-74	1.22166	6	1.22164	4
				<b>NISOT=18</b>		<b>NELEM=7</b>		<b>NMAT=4</b>	
ADS-ThU	300	1.18116 $\pm 29$		1.18033	-59	1.18033	0	1.18036	2
	1200	1.16175 $\pm 23$		1.16035	-104	1.16035	0	1.16036	1
	300v	1.21618 $\pm 28$		1.21504	-77	1.21505	0	1.21506	1
	1200v	1.19412 $\pm 24$		1.19377	-24	1.19378	1	1.1938	2
				<b>NISOT=25</b>		<b>NELEM=8</b>		<b>NMAT=4</b>	
ADS-XADS	300	1.40447 $\pm 28$		1.40298	-76	1.40297	0	1.40301	2
	1200	1.38989 $\pm 26$		1.38825	-85	1.38825	0	1.38827	1
	300v	1.53568 $\pm 30$		1.53456	-47	1.53460	1	1.53473	7
	1200v	1.52002 $\pm 33$		1.51958	-19	1.51960	1	1.51971	6
				<b>NISOT=26</b>		<b>NELEM=9</b>		<b>NMAT=4</b>	
xads_Bi	300	1.40791 $\pm 26$		1.40762	-15	1.40763	0	1.40757	-3
	1200	1.39403 $\pm 27$		1.39360	-22	1.39362	1	1.39356	-2
	300v	1.53568 $\pm 30$		1.53456	-47	1.53460	1	1.53473	7
	1200v	1.52002 $\pm 33$		1.51958	-19	1.51960	1	1.51971	6
				<b>NISOT=29</b>		<b>NELEM=12</b>		<b>NMAT=4</b>	
efr1	300	1.30074 $\pm 27$		1.30131	34	1.30142	7	1.30140	5
	1200	1.27944 $\pm 28$		1.28002	36	1.28013	7	1.28008	3
	300v	1.35236 $\pm 28$		1.35248	6	1.35257	5	1.35257	5
	1200v	1.33561 $\pm 26$		1.33536	-14	1.33545	5	1.33543	4
				<b>NISOT=11</b>		<b>NELEM=6</b>		<b>NMAT=3</b>	
molt	300	1.5843 $\pm 51$		1.58614	73	1.58617	2	1.58603	-4
	1200	1.51464 $\pm 53$		1.51837	162	1.51841	2	1.51842	2
	300v	1.13702 $\pm 48$		1.13944	186	1.13924	-15	1.13817	-98
	1200v	1.03124 $\pm 46$		1.02925	-187	1.02922	-3	1.02901	-23
				<b>NISOT=11</b>		<b>NELEM=7</b>		<b>NMAT=3</b>	
molt_U3	300	1.0815 $\pm 29$		1.08253	88	1.08253	0	1.08252	-1
	1200	1.08749 $\pm 27$		1.08818	58	1.08818	0	1.08819	1
	300v	0.99289 $\pm 43$		0.99735	450	0.9973	-2	0.99683	-52
	1200v	0.94051 $\pm 37$		0.94347	334	0.94346	-2	0.94344	-3
				<b>NISOT=22</b>		<b>NELEM=7</b>		<b>NMAT=4</b>	
scfbr1	300	1.19423 $\pm 38$		1.19554	92	1.19561	5	1.19611	40
	1200	1.15058 $\pm 35$		1.15001	-43	1.15011	8	1.15021	15
	300v	1.45372 $\pm 31$		1.4541	17	1.45406	-1	1.45420	5
	1200v	1.43976 $\pm 30$		1.43951	-12	1.43951	0	1.43960	4
				<b>NISOT=24</b>		<b>NELEM=8</b>		<b>NMAT=4</b>	
scfbr1_Cm	300	1.18056 $\pm 37$		1.18131	54	1.18138	5	1.18187	40
	1200	1.13714 $\pm 36$		1.13719	4	1.13729	8	1.1374	16
	300v	1.45723 $\pm 29$		1.45766	20	1.45765	-1	1.45781	7
	1200v	1.44414 $\pm 28$		1.44423	4	1.44423	0	1.44435	6

$\Delta K$  - MCNP  $1\sigma$  uncertainty     $\Delta IM$  = ISOT/MCNP-1 [pcm]     $\Delta EI$  = ELEM / ISOT-1 [pcm]     $\Delta MI$  = MAT/ ISOT-1 [pcm]

## 5.2 Performance of extended probability tables in the ACE files.

Validity of probabilistic representations in resolved resonance region has been tested in the SCERZO-556 homogeneous uranium media, which has been proposed as an international standard for intercomparison of experimental techniques and for the data testing. SCERZO-556 - imaged critical infinity composition of 5.56%  $^{235}\text{U}$  and 94.44%  $^{238}\text{U}$   $k$ -inf, evaluated on the base of a set of measurements of reactivity coefficients and spectral indexes in critical assemblies SNEAK, ERMINE and HARMONIE. The following characteristics for this infinity media were identified:  $k$ -inf =  $1.000 \pm 0.2\%$ ,  $F238/F235 = 0.0227 \pm 1.3\%$ ,  $C238/F235 = 0.1154 \pm 1.5\%$  [21]. Calculations were performed with MCNP code and the ACE cross section data files prepared by the GRUCON package from the ENDF/B-VII.1 evaluated data. The ACE files have been prepared in two modes, identified here as "UR" and "RR+UR". The "UR" mode means preparation by commonly used way, with point-wise cross-sections for resolved resonances and probability tables for unresolved resonance parameters. In the "RR+UR" mode, cross sections in the upper part of resolved resonance region (RR) have been average in some energy intervals, probability tables have been prepared and "glued" with tables in the unresolved resonance region. The cross-section, prepared in these two modes, are shown in Fig.10. A lower bound of the RR region has been defined at energies, where influence of correlations in subgroup cross-sections sequence in collisions become small. In Fig. 11, average lethargy increments per collision is compared with resonance structure in vicinity of the RR lower bound for each isotope.

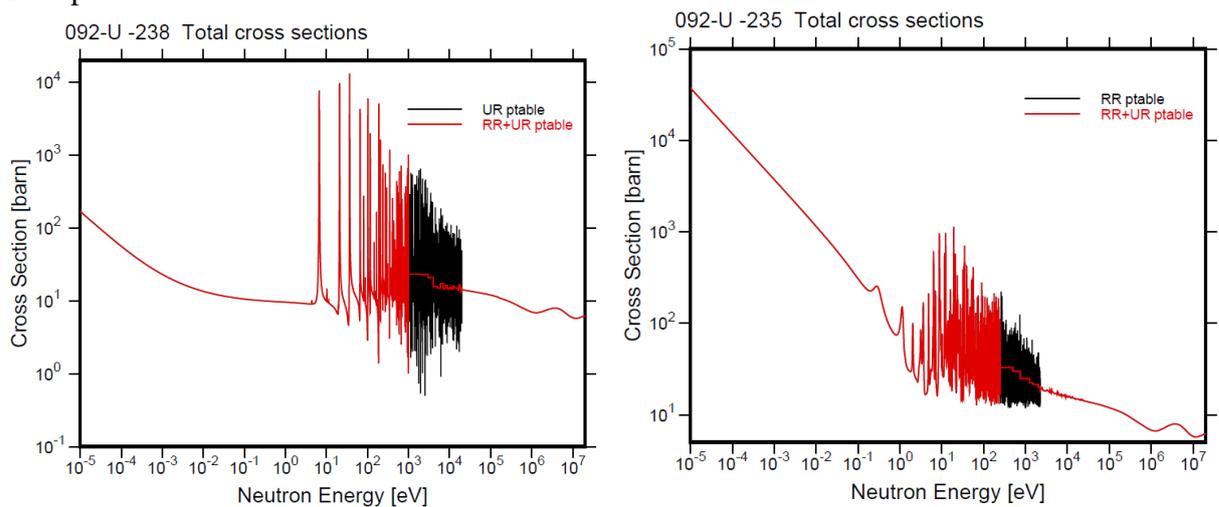


Fig.10 U-238 (left) и U-235 (right) total cross sections in UR and RR+UR data sets

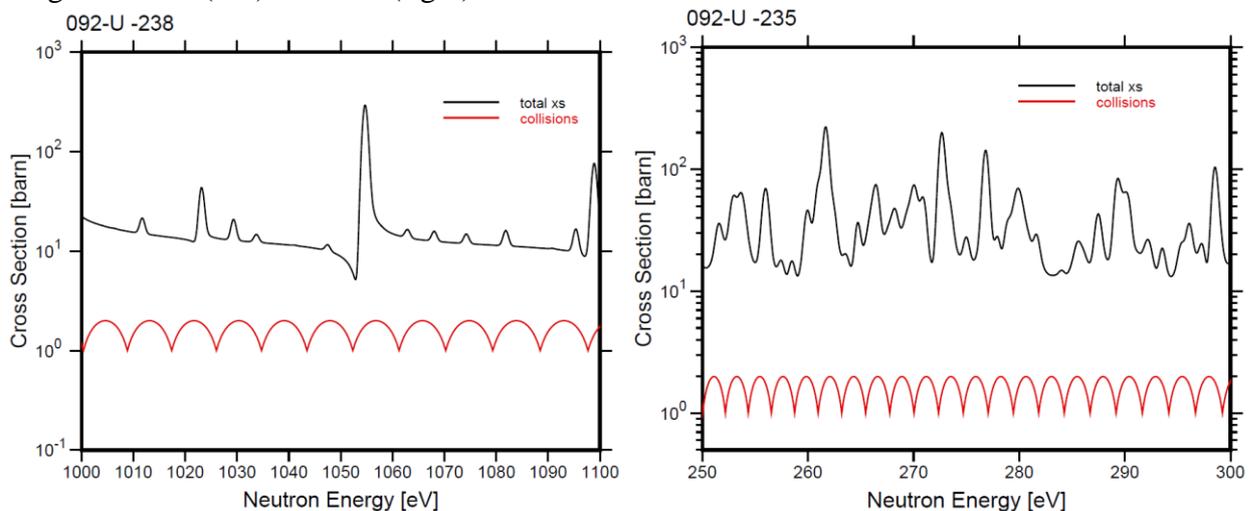


Fig.11 U-238(left) and U-235(right) total cross sections versus the average lethargy increment per collision

Four runs has been performed, with the different ACE files and the IUR calculation option:

- (A) ACE UR files, with probability table (IUR=0),
- (B) ACE RR+UR files, with probability tables (IUR=0),
- (C) ACE UR files, without probability tables (IUR=1),
- (D) ACE RR+UR files, without probability tables (IUR=1).

In Table 3 the results of experiment (E) and calculations ( $C_A$ ,  $C_B$ ,  $C_C$ ,  $C_D$ ) are compared. Statistical  $1\sigma$  errors ( in last figure) , experimental errors and C/E relative deviations ( in %) are given, to characterize:

- consistency with experiment ( $C_A/E-1$ ),
- validity of probabilistic approach to resonance structure presentations ( $C_B/C_A-1$ ),
- sensitivity to probability tables in the UR case,
- sensitivity to probability tables in the RR+UR case.

**Table 3. Kinf and reaction rate ratios for the SCHERZO-556 medium**

	Experiment	With probability tables ( IUR=0)			
		A: UR	( $C_A/E-1$ )%	B: RR+UR	( $C_B/C_A-1$ )%
<b>Kinf</b>	1.000 ± 0.2%	1.0008±(1)	0.08%	1.0009±(1)	<b>0.01%</b>
<b>F238/F235</b>	0.0227 ± 1.3%	0.02234±(1)	-1.6%	0.02233±(1)	<b>-0.04%</b>
<b>C238/F235</b>	0.1154 ± 1.5%	0.11552±(3)	0.1%	0.11552±(3)	<b>0.0%</b>
		Without probability tables ( IUR=1)			
		C: UR	( $C_C/C_A-1$ )%	D: RR+UR	( $C_D/C_B-1$ )%
<b>Kinf</b>		0.9904±(1)	- 1.0%	0.9860±(1)	<b>-1.5%</b>
<b>F238/F235</b>		0.02265±(1)	1.4%	0.02282±(1)	<b>2.2%</b>
<b>C238/F235</b>		0.11840±(3)	2.5%	0.11978±(3)	<b>3.7%</b>

As one can see, the  $C_A$  and  $C_B$  results coincide within statistical errors, which are substantially less experimental ones. The sensitivity of k-inf to probability tables in UR and RR+UR representations 0.96% and 1.4% correspondingly.

The relative size of the U235 and U238 ACE files in UR and RR+UR representations, is shown in Fig.12.

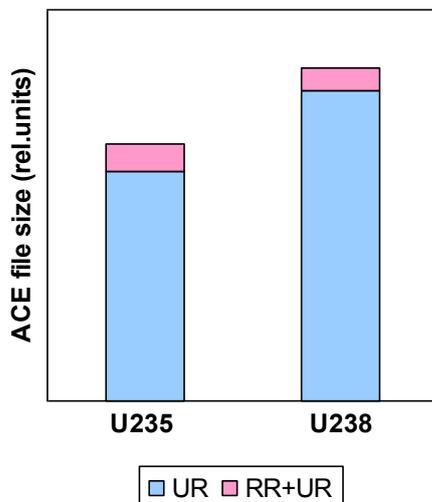


Fig.12 The ACE file volumes for U235 and U238 data in UR and RR+UR representations.

## Conclusion and Proposal

Probabilistic representations of the resonance cross sections structure allow take into account with required accuracy the most important resonance effects with significant ( tenfold ) decreasing in data volume and computing time consumption. It gives a possibility to solve complex computational tasks, in particular, of nuclear safety analyses.

The GRUCON code and C4R+C4P processing codes can supply the SIMMER and SAPHIR safety codes, as well as MCNP Monte Carlo transport code system, such type of data.

It is proposed to include more general (as compared with probability tables) probabilistic representations in reconstructed cross section element of the top level hierarchy for resolved and unresolved resonance regions.

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