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Abstract

For the first time, a resonance-parameter covariance matrix (RPCM) has been generated for ^{235}U in the resolved resonance region. The method used to produce this RPCM is the retroactive approach of the SAMMY code [1].

As reported elsewhere [2], a Reich-Moore resonance evaluation for ^{235}U had been performed in the energy range between 0 and 2.25 keV using SAMMY; a total of 3193 resonances, including the external levels, were identified. At the time that the evaluation was performed, the complete RPCM was not generated because of computer memory and storage limitations [3]. Subsequently, a procedure for retroactively creating RPCMs has been developed and implemented in the SAMMY code. This procedure is used to generate the RPCM for the ^{235}U parameters of the ENDF/B-VI evaluation.

KEYWORDS: ^{235}U, resonance parameter, retroactive, covariance matrix

1. Introduction

Most of the existing evaluated nuclear data files are missing the associated resonance parameter covariance matrices (RPCMs); the RPCMs affect the uncertainty estimation for nuclear applications. To accurately estimate the uncertainties on k_{eff} and other nuclear calculations, there is a need to retroactively generate covariance matrices for the already evaluated resonance parameters. To this end, we have generated a RPCM for ^{235}U retroactively and used it to compute group-wise cross section uncertainties and correlation matrices.

In the Reich-Moore formalism, each resonance of ^{235}U is described by five parameters (resonance energy, gamma width, neutron width, and two channel fission widths), for a total of 15,965 parameters [2]. The large number of resonance parameters leads to two technical issues when generating the RPCM: (a) the computer memory required to process the data and resonance parameters into the RPCM and (b) the data storage and the subsequent processing of the resulting covariance matrix [3].

The former issue has been resolved by using a 64-bit Alpha computer with 32 GB of memory, together with a related improvement in SAMMY that increased its maximum array size. The latter issue has been solved by modifying the covariance processing code PUFF-IV [4] to enable processing of large (~ 2-GB) covariance matrices.

Simultaneous fitting of all data sets is then accomplished via SAMMY, properly including the effect of the data covariance matrices. The set of experimental data used in the retroactive covariance evaluation of ^{235}U is shown in Table 1.

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Table 1: Experimental data sets used in the ^{235}U CM evaluation.

Reference	Energy range (eV)	Data description Refs. 5-13
Harvey [5]	0.4 – 68.0	Transmission at 18 m 0.03269 atom/barn 77 K
Harvey [5]	4.0 – 2250.0	Transmission at 80 m 0.00233 atom/barn 77 K
Harvey [5]	4.0 – 2250.0	Transmission at 80 m 0.03269 atom/barn 77 K
Schrack [6]	0.02 – 20.0	Fission at 18 m
de Saussure [7]	0.01 – 2250.0	Fission at 25.2 m
de Saussure [7]	0.01 – 2250.0	Capture at 25.2 m
Perez [8]	0.01 – 100.0	Fission at 39.7 m
Perez [8]	0.01 – 100.0	Capture at 39.7 m
Gwin [9]	0.01 – 20.0	Fission at 18.9 m
Spencer [10]	0.01 – 1.0	Transmission at 80 m 0.001468 atom/barn 77 K
Wagemans [11]	0.001 – 4.0	Fission at 18 m
Gwin [12]	0.01 – 4.0	Absorption
Gwin [12]	0.01 – 4.0	Fission
Weston [13]	14.0 – 2250.0	Fission at 18.9 m

2. Retroactive Covariance Matrix Method

The Bayesian iteration scheme for fitting the resonance parameters in SAMMY [1] gives the updated resonance parameter set (P') as

$$P' = P + M'Y \quad , \tag{1}$$

where the associated RPCM M' is found from

$$M' = (M^{-1} + W)^{-1} \qquad \text{with} \qquad W \equiv G^t V^{-1} G \quad , \tag{2}$$

and where Y is defined as an auxiliary matrix,

$$Y \equiv G^t V^{-1}(D - T) \quad . \tag{3}$$

In these equations, P represents the initial parameter set and M the associated RPCM, which in this case is unknown and therefore assumed to be diagonal and infinite; that is, $M^{-1} = 0$. The symbol V represents the data covariance matrix, T the theoretical value corresponding to the experimental data D, and G the theoretical sensitivity matrix,

$$G = \frac{\partial T}{\partial P} \quad . \tag{4}$$

The above equations are used to retroactively create a covariance matrix to be associated with a set of evaluated resonance parameters for which no covariance matrix had

previously been generated, as follows: By fitting to artificially generated data (D) with a realistic data covariance matrix (V) in the above equations, we are guaranteeing that $D = T$ in Eq. (3), from which it follows that $P' = P$ in Eq. (1). The parameter covariance matrix M', found in Eq. (2) as the RPCM associated with P', is therefore also appropriate for P. Hence we may use M' for the resonance parameter covariance matrix associated with the evaluated set of resonance parameters P.

3. Groupwise Covariance Matrix

Flux-weighted group cross sections are defined for a reaction cross section, for example σ_x, as

$$\bar{\sigma}_{xg}\,\Phi_g = \int_{E_g}^{E_{g+1}} \sigma_x(E)\,\Phi(E)\,dx \tag{5}$$

with

$$\Phi_g = \int_{E_g}^{E_{g+1}} \Phi(E)\,dx \quad . \tag{6}$$

Here Φ_g is the neutron flux in the energy group g, and $\bar{\sigma}_{xg}$ is the flux-weighted group cross section. The covariance matrix for the group cross section is obtained by taking small increments in $\bar{\sigma}_{xg}$ with respect to the resonance parameters, as

$$\delta\bar{\sigma}_{xg} = \sum_j \frac{\partial\sigma_{xj}}{\partial p_j}\,\delta p_j \quad . \tag{7}$$

The group covariance matrix elements are obtained as the expectation value of the product of two small increments, that is

$$\left\langle \delta\bar{\sigma}_{xg}\;\delta\bar{\sigma}_{xg'} \right\rangle = \sum_{jk} \frac{\partial\sigma_{xj}}{\partial p_j} \left\langle \delta p_j\;\delta p_k \right\rangle \frac{\partial\sigma_{xk}}{\partial p_k} \quad , \tag{8}$$

in which

$$\left\langle \delta p_j\;\delta p_k \right\rangle = M'_{jk} \tag{9}$$

is the retroactive covariance matrix element computed as described in Sect. 2. It is apparent from Eqs. (8) and (9) that the retroactive resonance parameter covariance matrix M' affects the group-averaged cross section covariance matrix, and consequently also affects the group-averaged cross section uncertainties.

The uncertainties on the group-averaged cross section are given by the square root of the diagonal elements of the group-averaged covariance matrix of Eq. (8). These cross sections and uncertainties are listed in Table 2 for the case of constant neutron flux ($\Phi(E) =$ constant). The corresponding correlation matrices, normalized to 100, are plotted in Figs. 1–3 for total, fission, and capture group-averaged cross sections, respectively.

Table 2: Average cross section (barn) and uncertainty calculated with SAMMY using the resonance parameter covariance matrix generated retroactively, assuming constant flux.

Energy range (eV)		Total cross section	Uncertainty in total cross section	Fission cross section	Uncertainty in fission cross section	Capture cross section	Uncertainty in capture cross section
.00001	0.003	4071.168	15.218	3407.827	12.628	646.715	14.415
0.003	0.008	1650.618	4.884	1376.397	4.281	258.869	5.097
0.008	0.010	1237.457	3.080	1031.508	3.078	190.689	3.388
0.010	0.025	873.532	1.799	729.868	2.103	128.494	2.082
0.025	0.030	665.692	1.250	557.352	1.576	93.238	1.506
0.030	0.040	583.922	1.073	488.672	1.384	80.187	1.325
0.040	0.050	504.164	0.919	421.056	1.204	68.094	1.158
0.050	0.070	425.239	0.784	353.380	1.023	56.915	0.982
0.070	0.100	342.878	0.653	281.918	0.837	46.125	0.789
0.100	0.150	271.497	0.563	218.771	0.682	38.058	0.630
0.150	0.200	231.802	0.538	181.492	0.598	35.840	0.561
0.200	0.225	228.180	0.575	175.086	0.614	38.759	0.611
0.225	0.250	238.152	0.620	181.234	0.659	42.646	0.694
0.250	0.275	250.848	0.679	190.675	0.705	45.927	0.769
0.275	0.325	244.944	0.685	187.997	0.661	42.668	0.729
0.325	0.350	209.115	0.609	162.424	0.552	32.397	0.570
0.350	0.375	181.480	0.517	141.573	0.492	25.643	0.460
0.375	0.400	158.914	0.433	124.098	0.444	20.601	0.380
0.400	0.625	107.885	0.274	82.833	0.304	11.116	0.237
0.625	1.000	78.647	0.216	58.113	0.225	7.143	0.178
1.000	1.770	61.380	0.201	38.116	0.180	10.275	0.185
1.770	3.000	33.353	0.153	13.852	0.116	7.316	0.118
3.000	4.750	40.220	0.173	18.572	0.120	10.085	0.139
4.750	6.000	43.472	0.198	13.231	0.124	19.299	0.180
6.000	8.100	79.538	0.253	24.473	0.168	44.115	0.262
8.100	10.00	171.748	0.435	116.899	0.433	43.026	0.423
10.00	30.00	88.292	0.188	43.637	0.127	32.942	0.157
30.00	100.00	65.824	0.160	35.164	0.098	18.765	0.103
100.00	550.00	36.293	0.149	16.666	0.053	7.787	0.088
550.00	2250.0	23.298	0.146	7.577	0.271	3.949	0.365

Figure 1: Correlation of the group-wise **<u>total cross section</u>** for the 30 energy groups spanning the ^{235}U resolved resonance region 0–2250 eV.

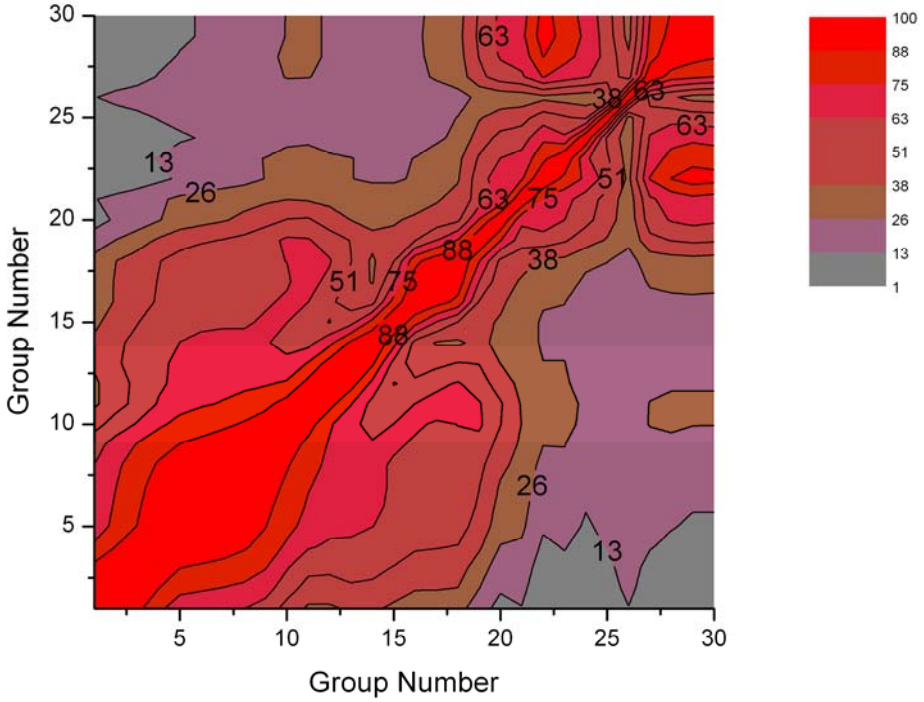


Figure 2: Correlation of the group-wise **<u>fission cross section</u>** for the 30 energy groups spanning the ^{235}U resolved resonance region 0–2250 eV.

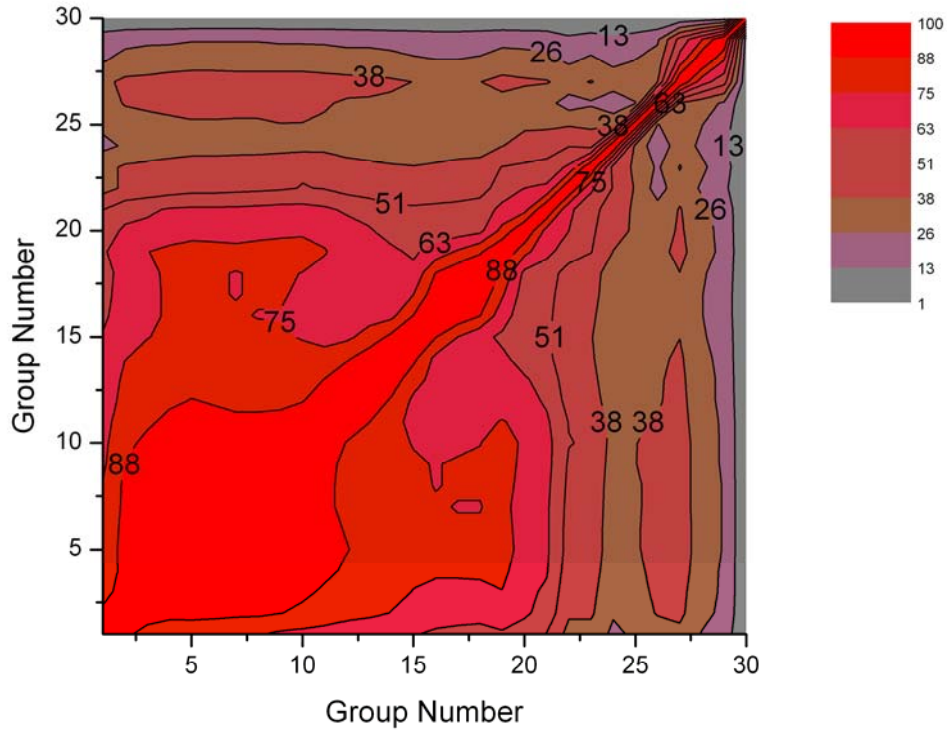
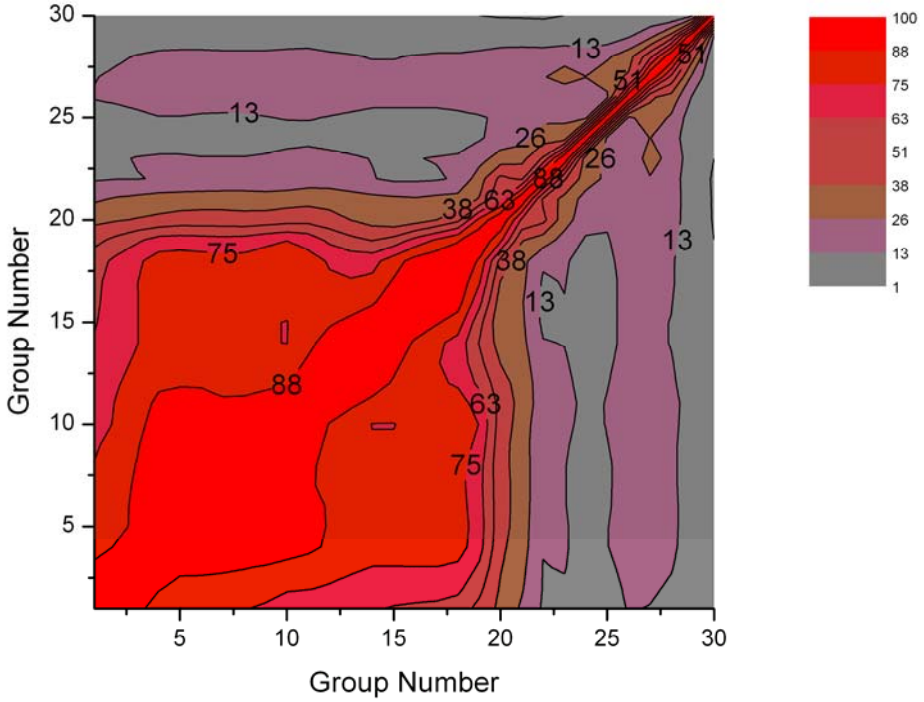


Figure 3: Correlation matrix for the group-wise **capture cross section** for 30 energy groups spanning the ^{235}U resolved resonance region 0–2250 eV.



4. Results and Conclusions

The retroactive procedure in SAMMY requires that the updated set of resonance parameters (P'), obtained after a single Bayes iteration, be nearly identical to the original set (P). To fulfill this requirement, the experimental data in each data set listed in Table 1 were replaced by theoretical values calculated from the evaluated resonance parameters via a no-Bayes SAMMY run. Experimental uncertainties from the original measurements were assigned as uncertainties on the calculated values that are now serving as artificial data.

For each data set created in the above fashion, the components of the off-diagonal data covariance matrix (DCM) were computed, including energy-dependent statistical uncertainties from the measurement and systematic uncertainties arising from normalization and background. Normalization and background corrections for the data listed in Table 1 were taken from Ref. 2.

A SAMMY run was then used to fit the artificial data, properly including the full off-diagonal DCM for each data set. This run produced the retroactive RPCM for the ^{235}U resonance parameters in the resolved-resonance region.

Average total, capture, and fission cross sections and their corresponding uncertainties have been calculated for the 30 low-energy groups in the 44-group structure of the SCALE system [14], spanning the entire resolved-resonance energy region of ^{235}U. The calculations, including the effect of the resonance-parameter covariance matrix, were performed with SAMMY. Results are shown in Table 2.

For the first time, a resonance parameter covariance matrix for ^{235}U has been generated for the resolved-resonance region. The evaluated RPCM will be submitted for inclusion in the ENDF library.

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