EXFOR compilation status in India and Uncertainty propagation in neutron activation cross section measurement using unscented transformation method

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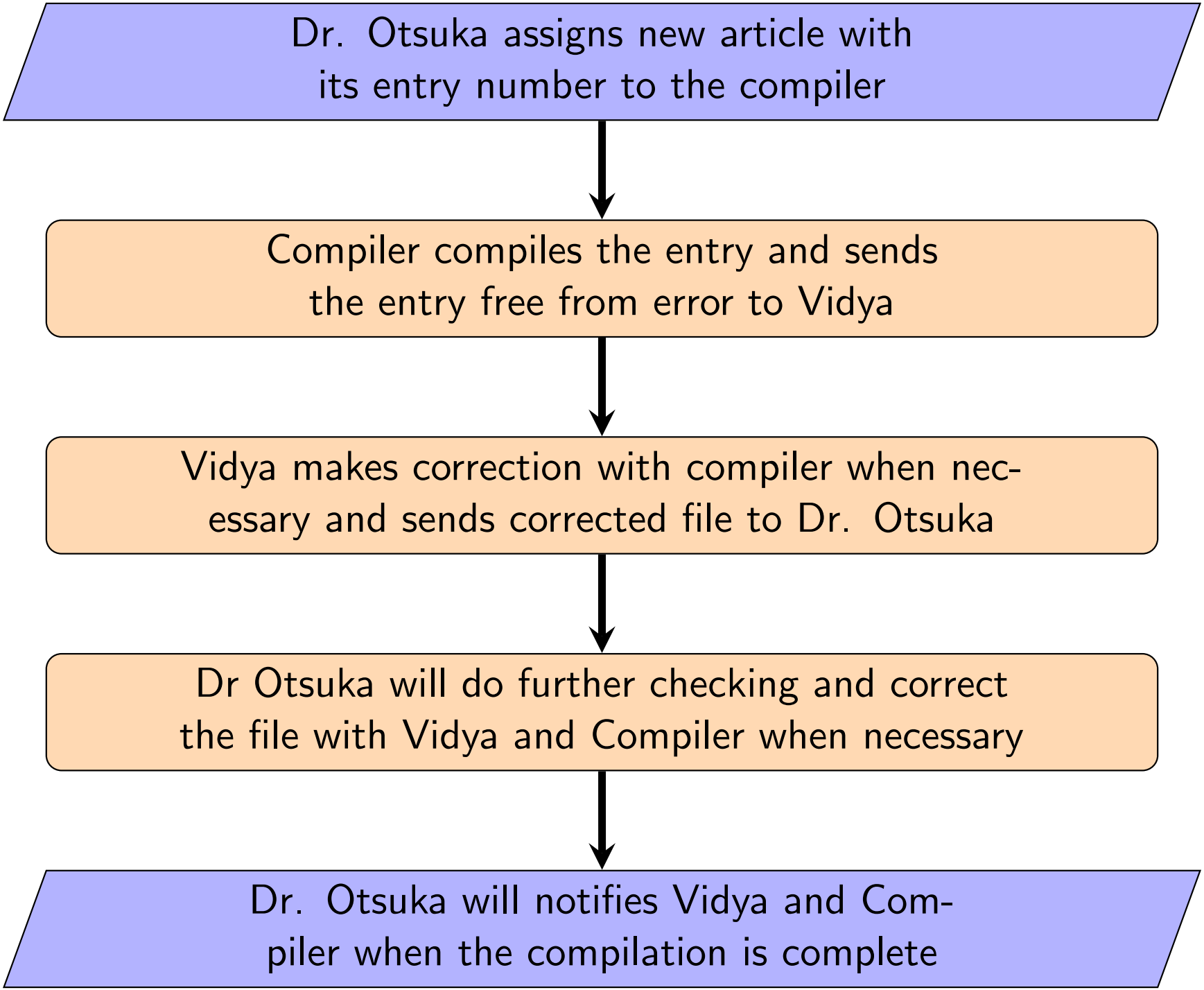
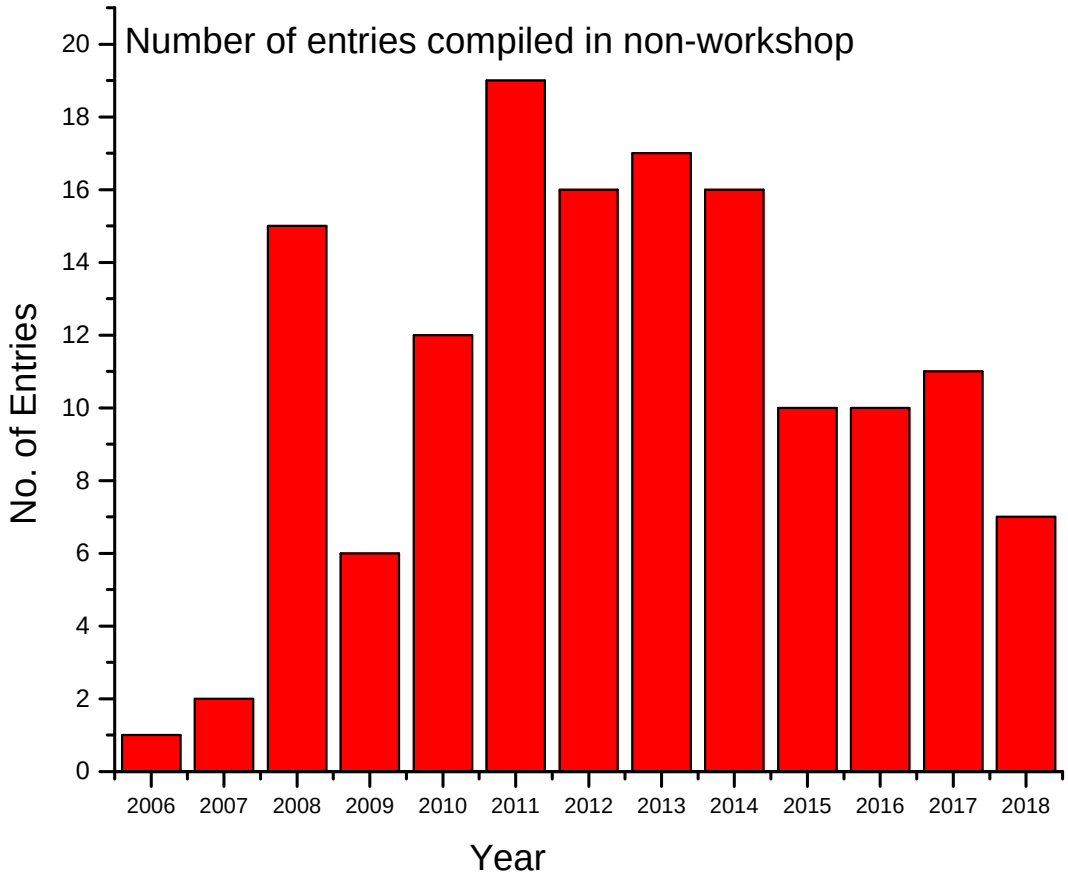
Content

- EXFOR compilation activities
- Uncertainty propagation in neutron activation cross section
- Conclusion

- In India, EXFOR compilation on a regular basis has been started since 2006.
- EXFOR compilation in INDIA is the outcome of the initiative and efforts undertaken by Nuclear Data Physics Centre of India (NDPCI).
- Since the past few years, EXFOR compilation has also been done by Universities through funds given by NDPCI-BRNS.
- All EXFOR compilations were done under the supervision of NDS, IAEA (Previously with the help of Dr. O. Schwerer, Dr. S. Dunaeva and currently with Dr. N. Otsuka).


Dr. Otsuka assigns new article with its entry number to the compiler
Compiler compiles the entry and sends the entry free from error to Vidya
Vidya makes correction with compiler when necessary and sends corrected file to Dr. Otsuka
Dr Otsuka will do further checking and correct the file with Vidya and Compiler when necessary
Dr. Otsuka will notifies Vidya and Compiler when the compilation is complete

Total number of entries for non-workshop or regular compilation activity since 2006



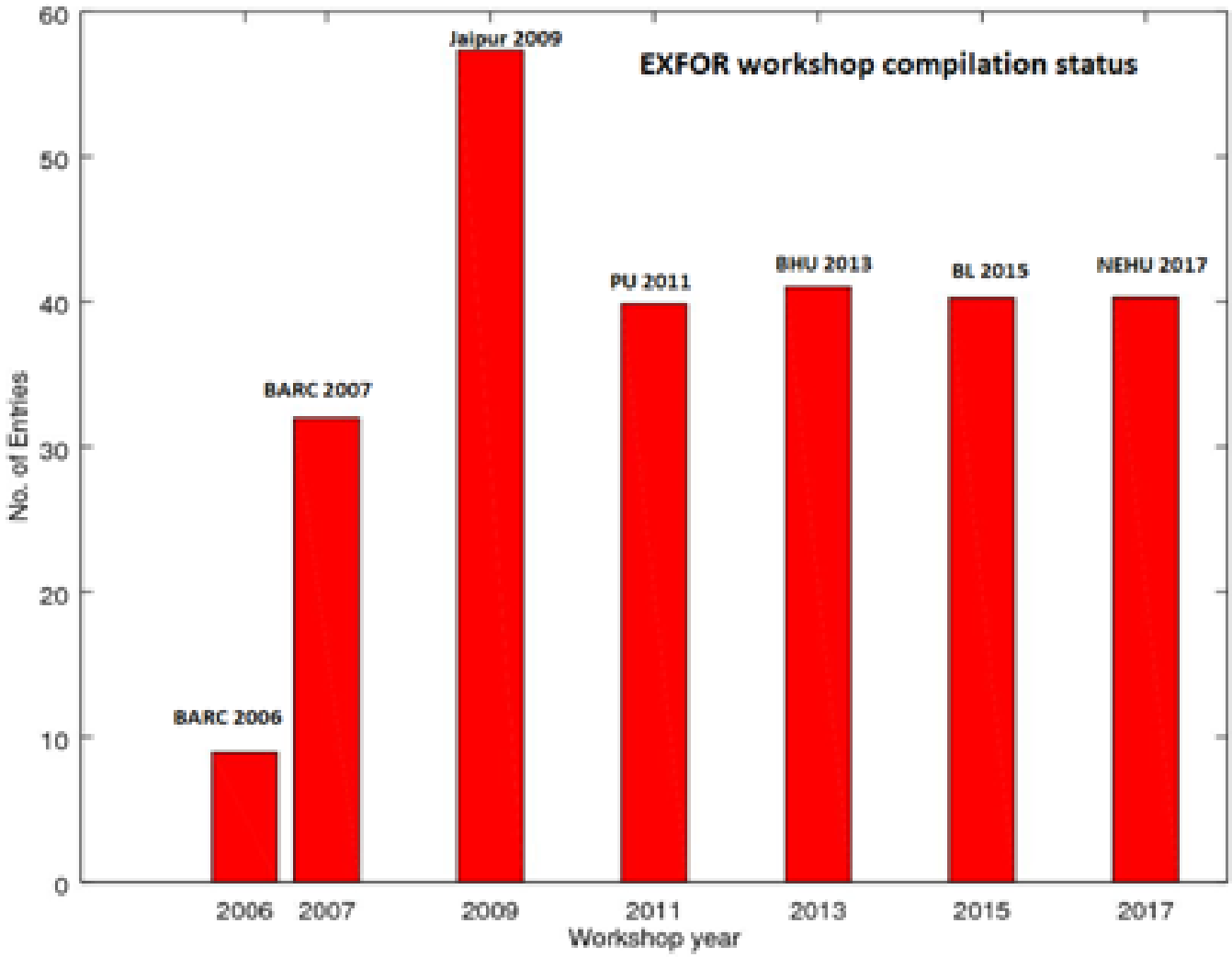
India successful contribution to the EXFOR entries by Workshop

- Before 2006 Indian experiments were directly compiled into EXFOR database by the IAEA staff.
- The 1st DAE-BRNS (Department of Atomic Energy-Board of Researches in Nuclear Sciences) theme meeting on EXFOR compilation of nuclear data was held in Mumbai(2006). In this meeting 10 new entries were finalized.
- The 2nd DAE-BRNS theme meeting on EXFOR compilation of nuclear data was held in Mumbai (2007). In this meeting 31 new entries were finalized under the supervision of Svetlana DUNAEVA with help of EXFOR editor.

- The 3rd DAE-BRNS theme meeting on EXFOR compilation of nuclear data was held in Jaipur (2009). In this meeting 55 new entries were finalized under the supervision of Svetlana DUNAEVA with help of EXFOR editor.
- The 4th DAE-BRNS theme meeting on EXFOR compilation of nuclear data was held in Punjab University Chandigarh (2011). In this meeting 40 new entries were finalized under the supervision of Svetlana DUNAEVA with help of EXFOR editor.
- The 5th DAE-BRNS theme meeting on EXFOR compilation of nuclear data was held in Banaras Hindu University. In this meeting 40 new entries were finalized under the supervision of N. Otsuka with help of EXFOR editor.

- The 6th DAE-BRNS theme meeting on EXFOR compilation of nuclear data will held in Bangalore from Jan. 20-24, 2015. In these meeting 40 new entries were finalized under the supervision of N. Otsuka with help of EXFOR editor.
- The 7th DAE-BRNS theme meeting on EXFOR compilation of nuclear data will held in Shillong from March 6-10, 2017. In these meeting 40 new entries were finalized under the supervision of N. Otsuka with help of EXFOR editor.
- The 8th DAE-BRNS theme meeting on EXFOR compilation of nuclear data will be held at university of Baroda 2019.

Total number of entries for workshop since 2006



Uncertainty propagation in neutron activation cross section

Understanding the structure of the atomic nucleus and developing a technology from the gained knowledge requires the experimental data and its uncertainties.

We mostly require physical quantities that cannot be directly measured and have to be calculated from variables that can be experimentally determined by using their functional dependence on each other.

We have to propagate the uncertainties of known variables to find the uncertainties of unknown variables. We will discuss two methodologies,

- Deterministic approach (Sandwich formula of error propagation and Unscented Transform Method)
- Stochastic approach (Monte Carlo method).

The Sandwich formula for error propagation is first order sensitivity analysis method. Let
x be an independent variable vector x of order n.
y be the dependent variable vector y of order m
Let $y{=}f(x)$ then the mean value of y is given as $\overline{y} \approx f(\overline{x})$.
The covariance matrix for Sandwich formula is given as

$$C_y \approx H_x C_x H_x^T. \tag{1}$$

Here C_x is $n \times n$ covariance matrix of x, C_y is $m \times m$ covariance matrix of y and H_x is the sensitivity matrix with elements $H_{xij} = \left(\frac{\partial f_i}{\partial x_j}\right)$
$(i = 1, 2, \ldots, m; j = 1, 2, \ldots, n)$.
This method works well for functions with small nonlinearity and small uncertainties but produces unsatisfactory results for higher nonlinearities.

Uncertainty propagation using Monte Carlo (MC) method:

Monte Carlo method is a stochastic approach that relies on repeated random sampling to obtain numerical results. Monte Carlo simulations are characterized by a large number of input vectors $\mathbf{x}^{(k)}$, $k = 1, 2, ..., K$, obtained by generating random numbers for each element x_i of $\mathbf{x}$

For each vector $\mathbf{x}^{(k)}$ produced, the m elements of vector $\mathbf{y}^{(k)}$ are calculated by the functional relationship $\mathbf{y} = \mathbf{f}(\mathbf{x})$.
From the large collection of derived vectors, sample mean values $\bar{\mathbf{y}}$ of K vectors can be estimated as

$$\bar{\mathbf{y}}_K = \frac{1}{K} \sum_{k=1}^{K} \mathbf{y}^{(k)} \tag{2}$$

Sample variances and covariances are given by

$$\mathbf{Cov} = \frac{1}{K} \sum_{k=1}^{K} \left(\mathbf{y}^{(k)} - \bar{\mathbf{y}}\right) \left(\mathbf{y}^{(k)} - \bar{\mathbf{y}}\right)^T. \tag{3}$$

Unscented Transform (UT) Method

- Unscented transform method is a deterministic method, easy to implement and does not require analytical linearization steps.
- It involves a set of points (called sigma points) has been generated that approximates the *pdf* of input parameters. These sigma points are transformed through the nonlinear function resulting in a set of transformed sigma points whom means and covariances are calculated.
- UT method sounds similar to the MC method, but has small set of vectors.

Unscented Transform (UT) Method

Let x be an $n \times 1$ vector with mean $\overline{x}$ and covariance P. In UT method we choose $2n$ sigma points $x^{(i)}$ as follow

$$x^{(i)} = \overline{x} + \widetilde{x}^{(i)}, \quad i = 1, 2, \ldots, 2n \tag{4}$$

where

$$\widetilde{x}^{(i)} = \left(\sqrt{nP}\right)_i^T, \quad \text{and} \quad \widetilde{x}^{(n+i)} = -\left(\sqrt{nP}\right)_i^T, \tag{5}$$

for $i = 1, 2, \ldots, n$. Here $\sqrt{nP}$ can be calculated using Cholesky factorization.
The mean and covariance using these sigma points are given by the formula

$$\overline{y} = \sum_{i=1}^{2n} W^{(i)} y^{(i)}, \qquad C = \sum_{i=1}^{2n} W^{(i)} \left(y^{(i)} - \overline{y}\right) \left(y^{(i)} - \overline{y}\right)^T.$$

$W^{(i)} = 1/2n, \ i = 1, 2, \ldots, 2n$ are weight coefficients.

Efficiency calibration of HPGe γ-ray detector

- In order to analyze uncertainty propagation methods, we have considered the experimental details of ^{58}Ni$(n,p)^{58}$Co reaction cross-sections relative to cross-section for the formation of ^{97}Zr fission product in neutron induced fission of ^{232}Th and ^{238}U at three effective incident neutron energies $E_n = 5.89$, 10.11 and 15.87 MeV are taken from research article of B. S. Shivashankar et.al [2015].
- In this experiment the efficiency of the detector is determined at six different energies of the calibration source ^{152}Eu given as:

$$\varepsilon = \frac{C}{A_o I_\gamma e^{\left(-\frac{0.693}{T_{1/2}} t\right)}} \tag{6}$$

Table: Experimental Counts values and Gamma Abundance [1]

γ-Energy (keV)	Counts per 900 seconds	γ-Abundance (%)
244.6975	10626 $\pm$ 193	7.583 $\pm$ 0.019
411.1163	1878 $\pm$ 110	2.234 $\pm$ 0.004
867.3780	1617 $\pm$ 95	4.245 $\pm$ 0.019
964.0790	5269 $\pm$ 100	14.605 $\pm$ 0.021
1112.074	4493 $\pm$ 89	13.644 $\pm$ 0.021
1299.140	510 $\pm$ 45	1.623 $\pm$ 0.008

Table: Mean value of detector efficiency(ε), standard deviation ($\delta\varepsilon$) and corresponding Covariance matrix ($\times 10^{-7}$) calculated using SA method.

SA method			
E_γ (keV)	ε%	$\delta\varepsilon$%	Covariance matrix ($\times 10^{-7}$)
244.675	3.3264	0.0902	8.147
411.116	1.9955	0.1236	2.656 15.268
867.378	0.9042	0.0563	1.203 0.722 3.165
964.079	0.8564	0.0236	1.140 0.686 0.309 0.560
1112.074	0.7817	0.0220	1.040 0.624 0.282 0.269 0.486
1299.140	0.7459	0.0676	0.992 0.595 0.270 0.256 0.233 4.568

Table: Mean value of detector efficiency(ε), standard deviation ($\delta\varepsilon$) and corresponding Covariance matrix ($\times 10^{-7}$) calculated using MC method.

MC method			
E_γ (keV)	$\delta\varepsilon$%	ε%	Covariance matrix ($\times 10^{-7}$)
244.675	3.3272	0.0904	8.172
411.116	1.9954	0.1236	2.646 15.260
867.378	0.9045	0.0562	1.206 0.710 3.161
964.079	0.8566	0.0237	1.146 0.686 0.309 0.560
1112.074	0.7819	0.0221	1.047 0.624 0.284 0.269 0.487
1299.140	0.7462	0.0677	0.997 0.586 0.267 0.256 0.234 4.589

Table: Mean value of detector efficiency(ε), standard deviation ($\delta\varepsilon$) and corresponding Covariance matrix ($\times 10^{-7}$) calculated using UT method.

UT method			
E_γ (keV)	$\delta\varepsilon$%	ε%	Covariance matrix ($\times 10^{-7}$)
244.675	3.3275	0.0905	8.218
411.116	1.9962	0.1244	2.699 15.292
867.378	0.9046	0.0561	1.223 0.734 3.171
964.079	0.8567	0.0236	1.158 0.695 0.315 0.564
1112.074	0.7820	0.0222	1.057 0.634 0.287 0.272 0.490
1299.140	0.7462	0.0677	1.009 0.605 0.274 0.260 0.237 4.571

- In SA method, sensitivities in efficiency are calculated in the form of partial derivatives of the $\varepsilon = \mathbf{f}(C, I_\gamma, A_o, T_{1/2})$ with respect to the four input random attributes to obtain the sensitivity coefficient matrix.
- In MC method, we generated $50,000$ normally distributed random numbers for each attribute (C, I_γ, A_o and $T_{1/2}$) having mean and standard deviation similar to input variables. Efficiencies were calculated for each gamma line corresponding to random variables.
- In UT method, we defined a primary variable vector with elements from four attributes for each γ-line. Eight sigma points were obtained for each input vectors and were transformed to 8 sigma points for transformed vectors.

Estimation of ^{58}Ni(n,p)^{58}Co reaction cross section

The activation cross section at a particular neutron energy for a reaction can be given as

$$\sigma = \frac{C\lambda}{N\Phi\varepsilon I(1 - e^{-\lambda t_{irr}})e^{-\lambda t_{cool}}(1 - e^{-\lambda t_{count}})}. \quad (7)$$

Here
C: Number of counts,
N: Number of atoms in the target,
Φ: the average Neutron flux in the target,
ε: detection efficiency of gamma ray detector
I: gamma radiation intensity
λ: decay constant
and t_{cool}, t_{count}, t_{irr} are cooling time, counting time, irradiation time, respectively. Usually, the direct measurement of Φ is avoided and is determined by using a monitor reaction (m) with monitor cross section (σ_m) value used from previous experiments or from data libraries [2, 3].

By substituting the value for Φ in Eq. (7) and rewriting it we get

$$\sigma_r = \sigma_m \frac{C_r \lambda_r N_m \varepsilon_m I_m (1 - e^{-\lambda_m t_{irr}}) e^{-\lambda_m t_{cool}} (1 - e^{-\lambda_m t_{count}}) \alpha_m}{C_m \lambda_m N_r \varepsilon_r I_r (1 - e^{-\lambda_r t_{irr}}) e^{-\lambda_r t_{cool}} (1 - e^{-\lambda_r t_{count}}) \alpha_r}, \tag{8}$$

where σ_r is the unknown cross-section for reaction $^{58}\mathrm{Ni}(n,p)^{58}\mathrm{Co}$ and σ_m is the cross-section for the fission yield of $^{97}\mathrm{Zr}$ in $^{232}\mathrm{Th}$ or $^{238}\mathrm{U}$ at neutron energy E_n. Here $\alpha_i,\ i = r, m$, is the flux energy correction factors. Some attributes, such as, t_{cool}, t_{count}, t_{irr}, α_r and α_m were observed without errors and treated as constants.

Sandwich formula

We have calculated the cross-section at three effective neutron energy E_n=5.89, 10.11 and 15.86 by substituting the basic data of attributes

$$(C_r, C_m, N_r, N_m, I_r, I_m, \lambda_r, \lambda_m, \sigma_m, Y, \varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)})$$

in Eq. (8).
The observation between any pair of attributes in Eq. (8) are independent of each other except $(\varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)})$. The correlation
Corr$(\varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)}) = 0.992$ between them. The corresponding output covariance matrix is calculated using sandwich formula by considering the mean value of input parameter and their correlations.

Defining Primary Variable Vector for UT and MC

Among the attributes mentioned in Eq. (8), we used attributes

$$(C_r, C_m, N_r, N_m, I_r, I_m, \lambda_r, \lambda_m, \sigma_m, Y, \varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)})$$

to define a primary variable vector

$$\mathbf{X}_j,\ j = 1, \ldots, 6$$

for each reaction (^{232}Th$(n,f)^{97}$Zr and ^{238}U$(n,f)^{97}$Zr) at three different effective neutron energies E_n =5.89, 10.11 and 15.87 MeV.

Cross section estimation using UT method

In UT method,

- we considered the primary variable vector $\mathbf{X}_j,\ j = 1, \ldots, 6$, as defined.
- The covariance matrix P_j is the block diagonal matrix of the form

$$P_j = \begin{pmatrix} P'_J & 0 \\ 0 & \mathbf{Cov}_{\varepsilon_\gamma} \end{pmatrix},$$

  where P'_j is the diagonal matrix with variances of the corresponding input parameters along the diagonal and $\mathbf{Cov}_{\varepsilon_\gamma}$ is the covariance matrix corresponding to the pair $(\varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)})$.
- We calculated 24 sigma points $\mathbf{X}_j^{(i)},\ i = 1, \ldots, 24$, for each input vector $\mathbf{X}_j,\ j = 1, \ldots, 6,$.
- These sigma points were transformed to the vectors

$$\sigma_{\mathbf{r_{UT}}}{}^{(i)} = (\mathbf{y}_1^{(i)}, \ldots, \mathbf{y}_6^{(i)}), i = 1, \ldots, 24,$$

  containing six elements (Cross-sections).
- Mean vector for transformed points and the corresponding covariance matrix were calculated using transformed vectors.

Table: $^{58}Ni(n,p)$ ^{58}Co reaction cross-section(σ_r) normalized with respect to $^{232}Th(n,f)$ $^{238}U(n,f)$ monitor cross-section and ^{97}Zr fission yield.

Monitor	Neutron energy (MeV)	SA Method		UT Method	
		σ_r	$\delta\sigma_r$	σ_r	$\delta\sigma_r$
Th	5.8883	0.43496	0.04774	0.43598	0.04880
U		0.52097	0.04256	0.52042	0.04237
Th	10.1126	0.59415	0.05609	0.59664	0.05674
U		0.67869	0.04270	0.67896	0.04245
Th	15.8673	0.18262	0.01852	0.18296	0.01799
U		0.19882	0.01559	0.19883	0.01542

Monte Carlo is similar to UT with large set of vectors

- we generated $50,000$ normally distributed random numbers for input parameters of primary variable vector $\mathbf{X}_j$ using code 'normrnd' of MATLAB except the pair $(\varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)})$.
- The pair $(\varepsilon_{\gamma(r)}, \varepsilon_{\gamma(m)})$ was fully correlated, hence, we generated $50,000$ correlated random numbers for them using MATLAB code 'mvnrnd'.
- The transformed vector ${\sigma_{\mathbf{r_{MC}}}}^{(i)} = (\mathbf{y}_1^{(i)}, \ldots, \mathbf{y}_6^{(i)}),\ i = 1, \ldots, 50000$, is obtained for cross section values for each reaction.
- Thereafter, sample mean and covariance matrix were calculated for the large set of output variables.

Table: $^{58}Ni(n,p)$ ^{58}Co reaction cross-section(σ_r) normalized with respect to $^{232}Th(n,f)$ $^{238}U(n,f)$ monitor cross-section and ^{97}Zr fission yield.

Monitor	Neutron energy (MeV)	MC Method		UT Method	
		σ_r	$\delta\sigma_r$	σ_r	$\delta\sigma_r$
Th	5.8883	0.43592	0.04818	0.43598	0.04880
U		0.52046	0.04210	0.52042	0.04237
Th	10.1126	0.59648	0.05560	0.59664	0.05674
U		0.67872	0.04235	0.67896	0.04245
Th	15.8673	0.18294	0.01795	0.18296	0.01799
U		0.19874	0.01547	0.19883	0.01542

- The deterministic SA method yields cross-section $\sigma_r = .43496$ with standard deviation $\delta\sigma_r = .04774$ for $^{232}\mathrm{Th}(n, f)$ at Neutron energy 5.8883 whereas the mean cross-section calculated using UT method is $\sigma_r = .43598$ with $\delta\sigma_r = .04880$.
- It can be seen that mean cross section calculated using UT method are closer to SA method upto 2 decimal places. The mean and standard deviations obtained using 24 sigma points in UT method are similar to mean and standard deviations calculated with MC method using 50,000 random variable. It is because of the advantage of UT being completely defined by the moments of higher order.

Table: Covariance matrix calculated using SA, MC and UT methods for cross section σ_r.

Covariance matrix ($\times 10^{-2}$) using SA method					
0.2280					
0.0976	0.1811				
0.0457	0.0023	0.3146			
0.0022	0.0203	0.1140	0.1824		
0.0140	0.0007	0.0192	0.0008	0.0343	
0.0006	0.0059	0.0008	0.0076	0.0178	0.0243
Covariance matrix ($\times 10^{-2}$) using MC method					
0.2226					
0.0945	0.1756				
0.0433	0.0011	0.3091			
0.0002	0.0185	0.1118	0.1793		
0.0136	0.0004	0.0188	0.0008	0.0322	
0.00008	0.0056	0.0004	0.0073	0.0178	0.0239

Table: Covariance matrix ($\times 10^{-2}$) using UT method for cross section σ_r.

Covariance matrix ($\times 10^{-2}$) using UT method					
0.2382					
0.1942	0.1795				
0.0372	0.0008	0.3220			
0.0009	0.0160	0.0955	0.2019		
0.0114	0.0003	0.0157	0.0004	0.0322	
0.0002	0.0047	0.0003	0.0061	0.0149	0.0238

Conclusion

- MC method provides the probability distribution for the cross sections that contains much more information but it can be difficult to extract those information. MC method is simple and easy to implement but have high computational time.
- The problem of high computation time and non-linear functions can be overcome by using UT method. Also, there is no need to calculate Jacobian matrix in UT method.
- Whenever non-linearity is high, Jacobian matrix is hard to calculate or micro-correlations are difficult to assign, UT method can serve as a great alternate to SA method for propagation of uncertainties.
- It will be of great interest to further examine the applications and performance of the UT method in complex reactor physics calculations.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THANKS FOR YOUR ATTENTION