SG39 Meeting
May 16-17, 2017

Update on Continuous Energy Cross Section Adjustment.

UC Berkeley / INL collaboration

Outline

- Presentation of the proposed methodology (you've already seen this)
- Results from ^{239}Pu adjustment from Jezebel integral experiment:
  - k_{eff}
  - F28/F25
  - F37/F25
  - F49/F25
- Comparison against ERANOS
- Conclusions

Continuous-energy first order uncertainty propagation

$$Var\left[R\right] = \int_{E_{min}}^{E_{max}} \int_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E)\,,\Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE' \tag{1}$$

$COV\left[\Sigma(E)\,,\Sigma(E')\right]$ is the continuous-energy covariance matrix

$S_{\Sigma}^{R}\left(E\right)$ is the sensitivity density function for the generic response R

Multi-group discretization is usually introduced here

Multi-group discretization of the covariance matrix

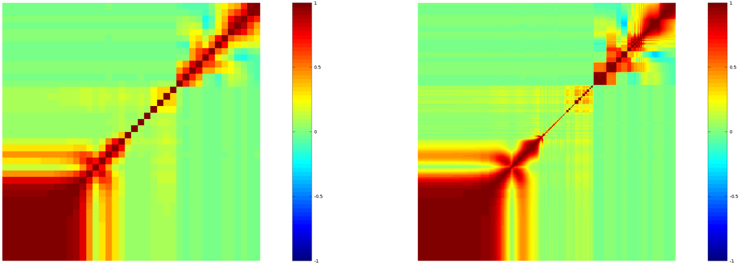


Figure: Comparison between the multi-group (left) and continuous (right) ^{239}Pu capture cross correlation matrices adopted in the adjustment process.

Multi-group discretization of the covariance matrix

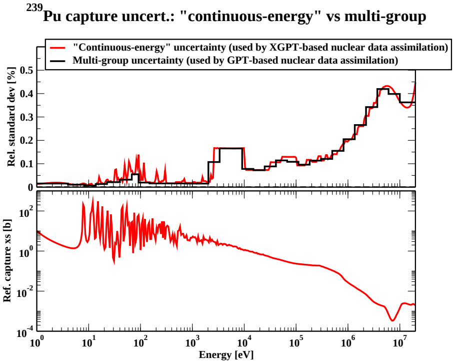


Figure: Comparison between ^{239}Pu capture cross section relative uncertainty adopted as input by the "continuous" and multi-group approaches.

Eigendecomposition of the covariance matrix

$$COV\left[\Sigma(E)\,,\Sigma(E')\right] = \sum_{j=1}^{\infty} U_j(E)\cdot V_j \cdot U_j(E') \quad (2)$$

V_j are the eigenvalues of the continuous energy covariance matrix corresponding to the eigenfunctions $U_j(E)$

Continuous-energy uncertainty propagation (revisited)

$$Var\left[R\right] = \int_{E_{min}}^{E_{max}} \int_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E)\, , \Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE' \tag{1}$$

$$Var\left[R\right] = \sum_{j=1}^{\infty} V_j \cdot \left(\int_{E_{min}}^{E_{max}} U_j\left(E\right) \cdot S_{\Sigma}^{R}\left(E\right)\, dE \right)^2 \tag{3}$$

Continuous-energy sensitivities

Main step: calculation of integral of continuous energy sensitivity functions via Monte Carlo XGPT:

$$S_{U_j}^{R} = \int U_j(E)\, S_{\Sigma}^{R}(E)\, dE$$

Continuous-energy uncertainty propagation (truncated)

$$Var\left[R\right] = \sum_{j=1}^{\infty} V_j \cdot \left(S^R_{U_j}\right)^2 \simeq \sum_{j=1}^{n} V_j \cdot \left(S^R_{U_j}\right)^2 \quad (4)$$

Projection vs. discretization

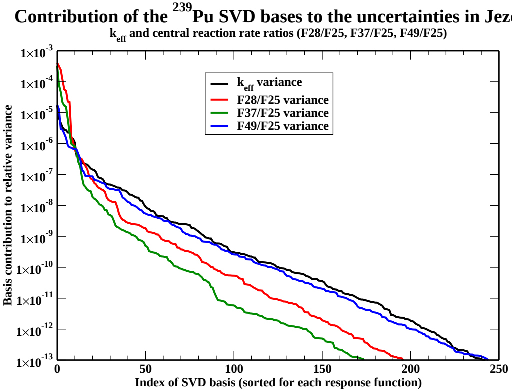


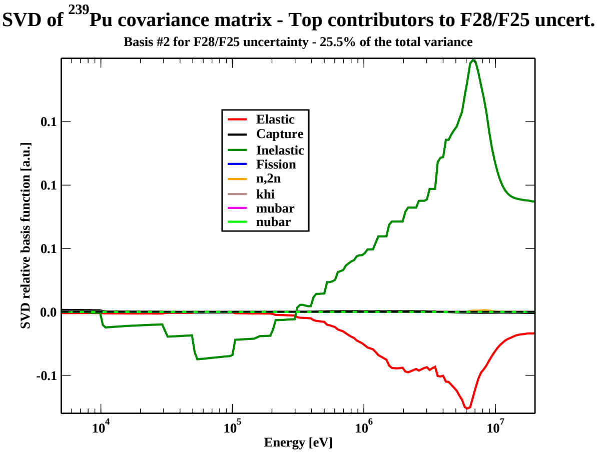
Figure: Eigenfunctions contribution to the total variances in Jezebel. Response functions: k_{eff} , F28/F25, F37/F25, F49/F25. (^{239}Pu ENDF/B-VII covariances).

Projection vs. discretization

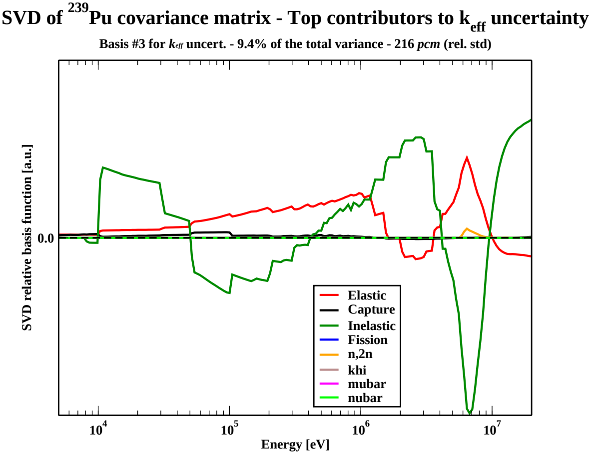
- Eigenvalue decomposition lead to exponential convergence with respect to the number of the basis functions
- Multi-group discretization lead to slow, unpredictable convergence with respect to the number of groups

- Statistical efficiency of Monte Carlo continuous sensitivity estimators doesn't depend on the number of eigenfunctions
- Statistical efficiency of Monte Carlo multi-group sensitivity estimators degrades quickly when adopting finer energy grids

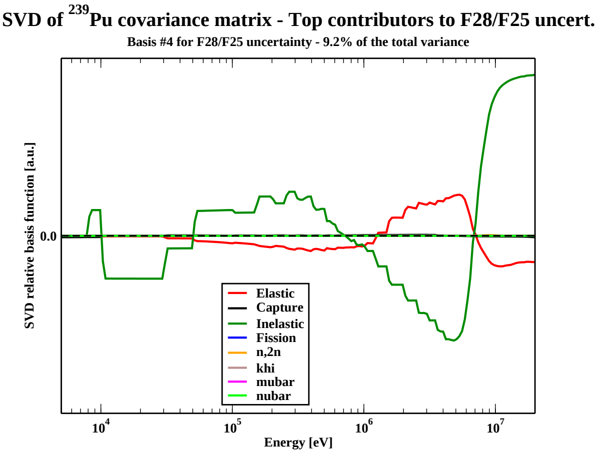
Example of basis functions from ^{239}Pu ENDF/B-VII



Example of basis functions from ^{239}Pu ENDF/B-VII



Example of basis functions from ^{239}Pu ENDF/B-VII



Multi-group/GPT starting point

Multi-group sensitivity coefficients:

$$\boldsymbol{S}_{\boldsymbol{\Sigma}}^{\boldsymbol{R}} = \left(S_{\Sigma_1}^{R}, S_{\Sigma_2}^{R} \cdots S_{\Sigma_N}^{R} \right) \tag{5}$$

Prior multi-group covariance matrices:

$$\boldsymbol{COV}\left[\boldsymbol{\Sigma}\ ,\boldsymbol{\Sigma}\right] = \begin{bmatrix} Var(\Sigma_1) & COV\left[\Sigma_1\ ,\Sigma_2\right] & \cdots & COV\left[\Sigma_1\ ,\Sigma_N\right] \\ COV\left[\Sigma_2\ ,\Sigma_1\right] & Var(\Sigma_2) & \cdots & COV\left[\Sigma_2\ ,\Sigma_N\right] \\ \vdots & \vdots & \ddots & \vdots \\ COV\left[\Sigma_N 1\ ,\Sigma_1\right] & COV\left[\Sigma_N\ ,\Sigma_1\right] & \cdots & Var(\Sigma_N) \end{bmatrix} \tag{6}$$

Continuous-energy/XGPT starting point

Eigenfunctions sensitivities:

$$\mathbf{S_U^R} = \left(S^R_{U_1}, S^R_{U_2} \cdots S^R_{U_n}\right) \tag{7}$$

Projection of the (prior) covariance matrices:

$$\mathbf{COV}\left[\mathbf{U}\ ,\mathbf{U}\right] = \begin{bmatrix} V_1 & 0 & \cdots & 0 \\ 0 & V_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V_n \end{bmatrix} \tag{8}$$

Continuous energy cross section adjustment

That's it!

S^R_Σ and $COV[\Sigma, \Sigma]$ are replaced by S^R_U and $COV[U, U]$

The continuous-energy adjustment process follows the standard, legacy multi-group approach...

Continuous energy cross section adjustment

Adjustment parameters $\mathbf{\Delta}_U = [\Delta_{U_1}, \Delta_{U_2} \cdots \Delta_{U_n}]^T$:

$$\mathbf{\Delta}_U = \mathbf{M}\,\mathbf{G}^T \left[\mathbf{G}\,\mathbf{M}\,\mathbf{G}^T + \mathbf{V_e} + \mathbf{V_m}\right]^{-1} \mathbf{D_R} \qquad (9)$$

- $\mathbf{M}$ is the prior covariance of the continuous functions ${}^{prior}\mathbf{COV}[\mathbf{U}\,,\mathbf{U}]$
- $\mathbf{V_e}$ and $\mathbf{V_m}$: matrices of the experimental and modeling errors
- $\mathbf{D_R}$ contains the relative differences between the calculated and measured experiments.
- $\mathbf{G}$ is the matrix of the sensitivities: $\mathbf{G} = \left[\mathbf{S_U^{R_1}} \mathbf{S_U^{R_2}} \cdots \mathbf{S_U^{R_N}}\right]^T$

Continuous energy cross section adjustment

$$\mathbf{\Delta}_U = \mathbf{M}\,\mathbf{G}^T \left[\mathbf{G}\,\mathbf{M}\,\mathbf{G}^T + \mathbf{V_e} + \mathbf{V_m}\right]^{-1} \mathbf{D_R} \quad (9)$$

$$^{adjusted}\Sigma\left(E\right) \simeq {}^{prior}\Sigma\left(E\right) \cdot \left(1 + \sum_{j=1}^{n} \Delta_{U_j} \cdot U_j\left(E\right)\right) \quad (10)$$

Adjusted continuous energy covariance

${}^{adjusted}\mathbf{COV}\left[\mathbf{U}\,,\mathbf{U}\right]$ via the Generalized Least Squares Method is obtained as:

$$
\begin{aligned}
&{}^{adjusted}\mathbf{COV}\left[\mathbf{U}\,,\mathbf{U}\right] - {}^{prior}\mathbf{COV}\left[\mathbf{U}\,,\mathbf{U}\right] = \\
&= \mathbf{M}\,\mathbf{G}^{T}\left[\mathbf{G}\,\mathbf{M}\,\mathbf{G}^{T} + \mathbf{V_e} + \mathbf{V_m}\right]^{-1}\,\mathbf{G}\,\mathbf{M}
\end{aligned}
\tag{11}
$$

${}^{adjusted}\mathbf{COV}\left[\mathbf{U}\,,\mathbf{U}\right]$ contains the correlations among the basis functions introduced by the experiments.

$$
\begin{aligned}
&{}^{adjusted}COV\left[\Sigma(E)\,,\Sigma(E')\right] \simeq \\
&\simeq \left[U_1(E) \quad \dots \quad U_n(E)\right]\;{}^{adjusted}\mathbf{COV}\left[\mathbf{U}\,,\mathbf{U}\right]\begin{bmatrix} U_1(E') \\ \vdots \\ U_n(E') \end{bmatrix}
\end{aligned}
\tag{12}
$$

Case study: Jezebel ^{239}Pu

Relative experimental uncertainties

k_{eff}	F28/F25	F37/F25	F49/F25
0.002	0.011	0.014	0.009

Experimental correlation matrix

	k_{eff}	F28/F25	F37/F25	F49/F25
k_{eff}	1.00	0.00	0.00	0.00
F28/F25	0.00	1.00	0.32	0.23
F37/F25	0.00	0.32	1.00	0.23
F49/F25	0.00	0.23	0.23	1.00

Table: Experimental uncertainties and correlation matrix for the four considered response functions.

Case study: Jezebel ^{239}Pu

Relative modeling uncertainties

k_{eff}	F28/F25	F37/F25	F49/F25
0.0018	0.0090	0.0030	0.0030

Modeling correlation matrix

	k_{eff}	F28/F25	F37/F25	F49/F25
k_{eff}	1.00	0.00	0.00	0.00
F28/F25	0.00	1.00	0.50	0.50
F37/F25	0.00	0.50	1.00	0.50
F49/F25	0.00	0.50	0.50	1.00

Table: Modeling uncertainties and correlation matrix for the four considered response functions.

Case study: Jezebel ^{239}Pu

	Exp.	Calc. (this work)	Calc. (WPEC-SG33)
k_{eff}	1.0000	0.99976	0.99986
F28/F25	0.2133	0.20871	0.20839
F37/F25	0.9835	0.97155	0.97071
F49/F25	1.4609	1.42435	1.42482

Table: Experimental and calculated values.

Continuous vs. multi-group: uncertainty reduction

	Prior rel. uncert. (%)		Post rel. uncert. (%)	
	multi-group	XGPT	multi-group	XGPT
k_{eff}	0.733	0.704	0.191	0.190
F28/F25	3.731	3.581	1.298	1.291
F37/F25	3.631	3.573	1.307	1.306
F49/F25	0.825	0.797	0.558	0.547

Table: Comparison of prior (input) and post (adjusted) nuclear data uncertainties estimated by the multi-group and continuous approaches for the four response functions.

Continuous vs. multi-group: uncertainty reduction

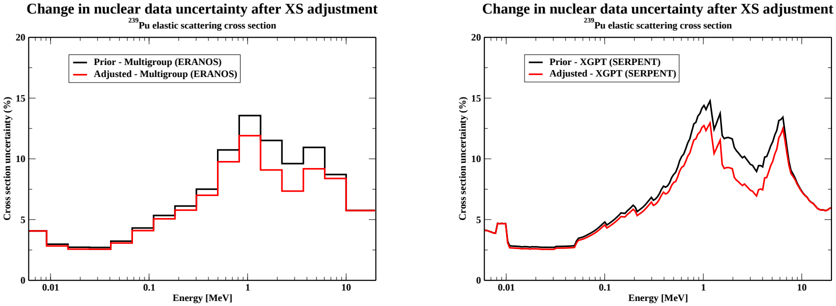


Figure: ^{239}Pu elastic scattering uncertainty before and after the adjustment process. Multi-group (left) and continuous energy (right) results.

Continuous vs. multi-group: uncertainty reduction

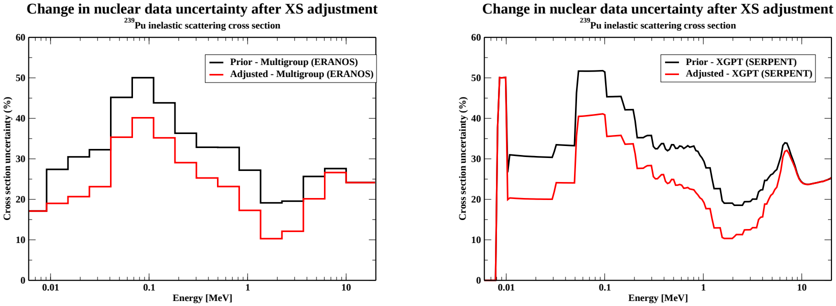


Figure: ^{239}Pu inelastic scattering uncertainty before and after the adjustment process. Multi-group (left) and continuous energy (right) results.

Negative correlations

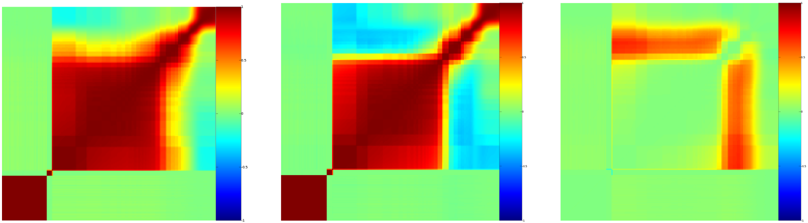


Figure: ^{239}Pu inelastic scattering correlation matrix in the 1 keV – 20 MeV energy region. Before (left) and after (center) the continuous energy adjustment process, and Prior – Post difference is shown on the right.

Continuous vs. multi-group: XS adjustment

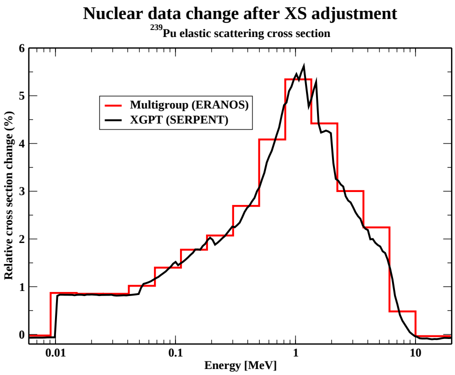


Figure: ^{239}Pu elastic scattering cross section before and after the adjustment process. Multi-group (red) and continuous energy (black) results.

Continuous vs. multi-group: XS adjustment

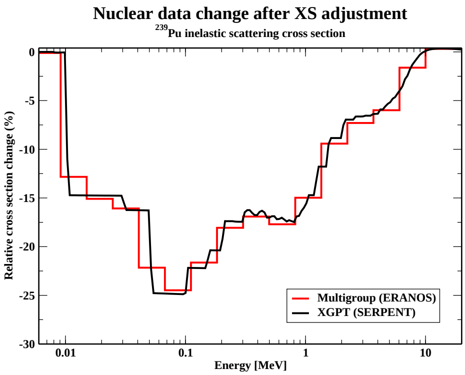


Figure: ^{239}Pu inelastic scattering cross section before and after the adjustment process. Multi-group (red) and continuous energy (black) results.

Continuous vs. multi-group: Post C/E

	Prior C/E		Post C/E	
	multi-group [1]	XGPT	multi-group	XGPT
k_{eff}	0.99986	0.99976	1.00001	1.00000
F28/F25	0.977	0.979	0.995	0.995
F37/F25	0.987	0.988	0.996	0.996
F49/F25	0.975	0.975	0.985	0.984

Table: Comparison of prior and post C/E estimated by the multi-group and continuous approaches for the four response functions.

Conclusions

Main goal: new methodology for continous-energy XS adjustment

Shorten the distance between evaluators and Monte Carlo users (?)

Enable the adoption of integral experiments in a simple, effective and timely way (^{35}Cl (n, p), ^{233}U (n, γ)...)

Conclusions

Main goal: new methodology for continous-energy XS adjustment

Shorten the distance between evaluators and Monte Carlo users (?)

Enable the adoption of integral experiments in a simple, effective and timely way (^{35}Cl (n,p), ^{233}U (n,γ)...)

First tests are promising... we need to move to broader case studies. **Anyone wants to help/contribute???**

In the resonance region, resonance parameters XS sensitivities (after MF-32 decompositions) and scattering radii are the basis functions for the continuous adjustment

Lessons learned (random thoughts) and ongoing works

- Please, leave MF-32 in the ENDF files
- In the future, storing MF-33 in the form of eigenvectors/eigenvalues might save, memory, CPU, and headaches
- Now working on secondaries distribution adjustment... Legendre or double differential?
- Next step: URR adjustment (this might take some time!)

Questions? Suggestions? Ideas?