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Fission Spectrum Covariance Matrix and Sensitivity Coefficients for Response Parameter Uncertainty Estimation

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Background

- The impact of the fission spectrum uncertainty on the multiplication factor uncertainty was previously investigated for the sodium-cooled ABTR and the KRITZ thermal benchmark experiment
  - G. Aliberti, I. Kodeli, G. Palmiotti, M. Salvatores, “Fission Spectrum Related Uncertainties,” NEMEA-4 Conference, Prague, October 16-18, 2007
- Significantly high uncertainties (~4%) were reported
  - Such high uncertainties exceed the typical uncertainties associated with the cross sections, and would impose important restrictions on the reactor design
- Inconsistencies in the sensitivity calculation methods and/or in the covariance matrix evaluation and processing were suggested as a possible explanation for the high uncertainties
- To clarify the differences in the sensitivity methodologies, a computational exercise was also performed
  - ERANOS, SAGEP and SUSD3D codes

Outline

- Covariance matrix in File 35 of ENDF
  - Properties
  - Normalization scheme
- Sensitivity coefficient calculation methods
  - Unconstrained sensitivity coefficients
  - Constrained sensitivity coefficients
- Equivalence of unconstrained and constrained sensitivity coefficients
  - Response parameter variation
  - Response parameter uncertainty
- Numerical Results
  - Sodium-cooled ABTR
- Conclusions

Properties of Covariance Matrix in File 35

- Fission spectrum

$$\sum_{i=1}^{n} \chi_i = 1$$

$$\mathbf{u}^T \boldsymbol{\chi} = \boldsymbol{\chi}^T \mathbf{u} = 1, \quad \mathbf{u} = (1,1,\cdots,1)^T$$

- Covariance matrix

$$\sigma_{ij} = (\mathbf{V}_\chi)_{ij} =< (\chi_i - \overline{\chi}_i)(\chi_j - \overline{\chi}_j) >$$

  – Symmetric
  – Positive definite
  – Zero column or row sum

$$\sum_{i=1}^{n} \sigma_{ij} = 0 \ \text{ or } \ \sum_{j=1}^{n} \sigma_{ij} = 0$$

Renormalization of Covariance Matrix in File 35

- Normalization scheme specified in File 35 of ENDF

$$\tilde{\sigma}_{ij} = \sigma_{ij} - \chi_i \sum_k \sigma_{kj} - \chi_j \sum_k \sigma_{ki} + \chi_i \chi_j \sum_k \sum_l \sigma_{kl}$$

- Congruent transformation

$$\tilde{\sigma}_{ij} = \sum_k \sum_l (\delta_{ki} - \chi_i) \sigma_{kl} (\delta_{lj} - \chi_j)$$

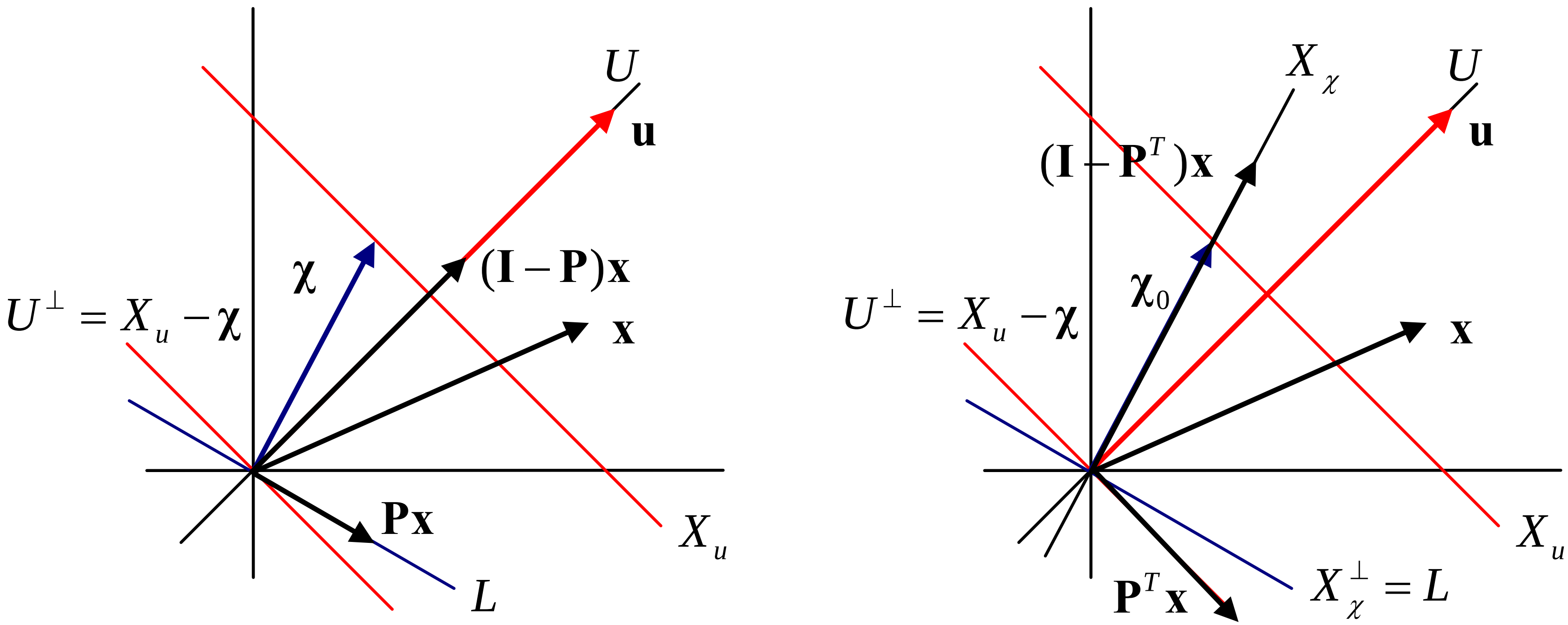
$$\tilde{\mathbf{V}}_\chi = \mathbf{P}^T \mathbf{V}_\chi \mathbf{P}$$

$$\mathbf{P} = \mathbf{I} - \mathbf{u}\boldsymbol{\chi}^T$$

  – $\mathbf{P}$ is an oblique projection operator
    - *Range:* $L = \{\mathbf{x} \in \mathbb{R}^n \mid \boldsymbol{\chi}^T \mathbf{x} = 0\}$
    - *Null space:* $U = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} = \alpha \mathbf{u}, \alpha \in \mathbb{R}\}$

$$\mathbf{P}^2 = \mathbf{P}$$

Properties of Projection Operator



$$L = \{\mathbf{x} \in \mathbb{R}^n \mid \boldsymbol{\chi}^T\mathbf{x} = 0\}$$

$$U = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} = \alpha\mathbf{u}, \alpha \in \mathbb{R}\}$$

$$X_u = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{u}^T\mathbf{x} = 1\}$$

$$U^{\perp} = X_u - \boldsymbol{\chi}$$

$$X_\chi = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} = \alpha\boldsymbol{\chi}, \alpha \in \mathbb{R}\}$$

$$X_\chi^{\perp} = L$$

Variation and Uncertainty of Response

- Variation of a response

$$\delta R = R(\boldsymbol{\chi}') - R(\boldsymbol{\chi}) = \nabla R(\boldsymbol{\chi}) \cdot (\boldsymbol{\chi}' - \boldsymbol{\chi}) = \mathbf{s}_\chi^T \delta\boldsymbol{\chi}$$

$$\mathbf{s}_\chi = \nabla R(\boldsymbol{\chi}) = \left(\frac{\partial R}{\partial \chi_1}, \frac{\partial R}{\partial \chi_2}, \cdots, \frac{\partial R}{\partial \chi_n} \right)^T$$

- Uncertainty of a response

$$\sigma_R^2 = < (\delta R)^2 > = \mathbf{s}_\chi^T < (\delta\boldsymbol{\chi})(\delta\boldsymbol{\chi})^T > \mathbf{s}_\chi = \mathbf{s}_\chi^T \mathbf{V}_\chi \mathbf{s}_\chi$$

$$\mathbf{V}_\chi = < (\delta\boldsymbol{\chi})(\delta\boldsymbol{\chi})^T >$$

Sensitivity Coefficients

- Unconstrained sensitivity coefficients
  - Gradient of a response at the point of nominal fission spectrum

$$\mathbf{s}_{\chi} = \nabla R(\boldsymbol{\chi}) = \left(\frac{\partial R}{\partial \chi_1}, \frac{\partial R}{\partial \chi_2}, \cdots, \frac{\partial R}{\partial \chi_n} \right)^T$$

- Constrained sensitivity coefficients (SAGEP of JAEA)
  - Perturbed fission spectrum is constrained to satisfy the fission spectrum normalization condition
  - Equivalent to the projection of the gradient on the surface representing the fission spectrum normalization condition

$$\tilde{\mathbf{s}}_{\chi} = \mathbf{P}\mathbf{s}_{\chi}$$

Equivalence of Constrained and Unconstrained Sensitivity Coefficients for Response Parameter Uncertainty Evaluation

- Response variation computed with constrained sensitivity coefficients

$$\delta R = \tilde{\mathbf{s}}_\chi^T \delta\boldsymbol{\chi} = (\mathbf{P}\mathbf{s}_\chi)^T \delta\boldsymbol{\chi} = \mathbf{s}_\chi^T \mathbf{P}^T \delta\boldsymbol{\chi} = \mathbf{s}_\chi^T \delta\boldsymbol{\chi}$$

- Response uncertainty computed with constrained sensitivity coefficients

$$\sigma_R^2 = \tilde{\mathbf{s}}_\chi^T \mathbf{V}_\chi \tilde{\mathbf{s}}_\chi = (\mathbf{P}\mathbf{s}_\chi)^T \mathbf{V}_\chi (\mathbf{P}\mathbf{s}_\chi) = \mathbf{s}_\chi^T \mathbf{P}^T \mathbf{V}_\chi \mathbf{P}\mathbf{s}_\chi = \mathbf{s}_\chi^T \tilde{\mathbf{V}}_\chi \mathbf{s}_\chi$$

$$\tilde{\mathbf{V}}_\chi = \mathbf{P}^T \mathbf{V}_\chi \mathbf{P}$$

  – Equivalent to normalizing the covariance matrix to satisfy the zero-sum constraint

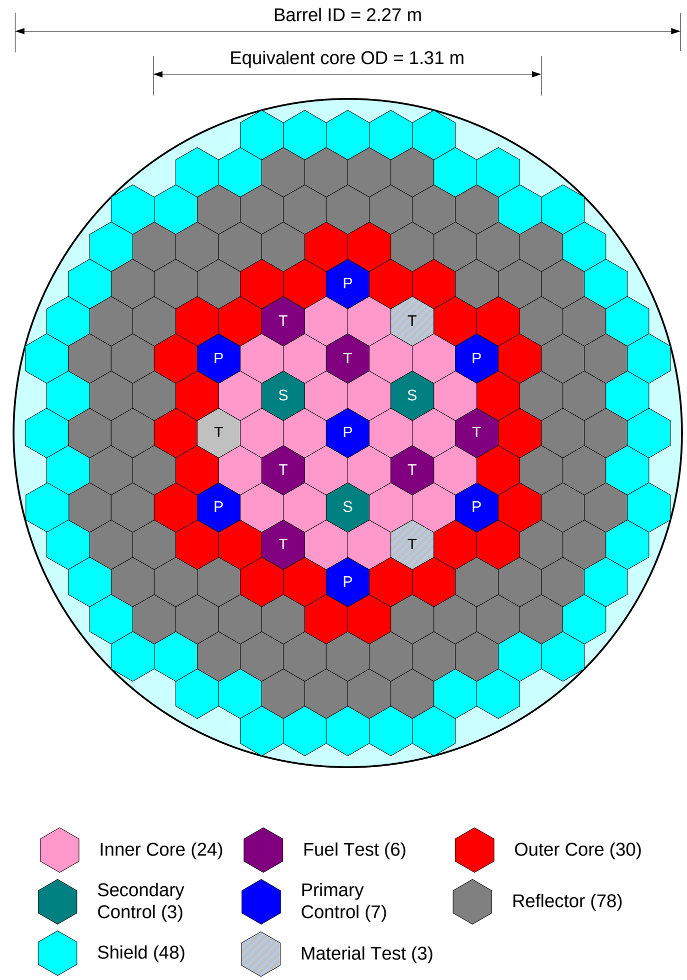
$$\mathbf{P}^T \tilde{\mathbf{V}}_\chi \mathbf{P} = (\mathbf{P}^T)^2 \mathbf{V}_\chi \mathbf{P}^2 = \mathbf{P}^T \mathbf{V}_\chi \mathbf{P} = \tilde{\mathbf{V}}_\chi$$

  – When a covariance matrix satisfies the zero sum constraint as required, constrained and unconstrained sensitivity coefficients yield the same uncertainty

Numerical Results

- Uncertainty of ABTR multiplication factor due to Pu-239 fission spectrum uncertainty

Energy group	Upper boundary (keV)	Fission spectrum	Sensitivity coefficients	
			unconstrained	constrained
1	19600	0.03089	0.0324	0.0081
2	6070	0.33969	0.2949	0.0253
3	2230	0.23100	0.1880	0.0042
4	1350	0.28041	0.2008	-0.0215
5	498	0.08958	0.0601	-0.0108
6	183	0.02192	0.0137	-0.0038
7	67.4	0.00505	0.0028	-0.0012
8	24.8	0.00113	0.0006	-0.0003
9	9.12	0.00029	0.0002	-0.0001
10	2.03	0.00003	0.0000	0.0000
11	0.454	0.00000	0.0000	0.0000
12	0.0226	0.00000	0.0000	0.0000
13	0.0040	0.00000	0.0000	0.0000
14	0.00054	0.00000	0.0000	0.0000
15	0.00010	0.00000	0.0000	0.0000
Total		1.00000	0.7935	0.0000



Un-normalized Covariance Matrix

Uncertainty (%)	Correlation															
	Gr.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
9.69	1	1.000	0.846	-0.326	-0.923	-0.671	-0.608	-0.590	-0.587	-0.587	-0.587	-0.590	-0.593	-0.593	-0.593	-0.593
3.47	2	0.846	1.000	0.227	-0.986	-0.963	-0.937	-0.929	-0.928	-0.928	-0.928	-0.930	-0.931	-0.931	-0.931	-0.931
1.03	3	-0.326	0.227	1.000	-0.062	-0.482	-0.552	-0.571	-0.574	-0.574	-0.574	-0.571	-0.568	-0.568	-0.568	-0.568
2.71	4	-0.923	-0.986	-0.062	1.000	0.905	0.867	0.855	0.853	0.853	0.853	0.855	0.857	0.857	0.857	0.857
5.36	5	-0.671	-0.963	-0.482	0.905	1.000	0.997	0.995	0.994	0.994	0.994	0.995	0.995	0.995	0.995	0.995
6.34	6	-0.608	-0.937	-0.552	0.867	0.997	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.73	7	-0.590	-0.929	-0.571	0.855	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.44	8	-0.587	-0.928	-0.574	0.853	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.73	9	-0.587	-0.928	-0.574	0.853	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.42	10	-0.587	-0.928	-0.574	0.853	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.44	11	-0.590	-0.930	-0.571	0.855	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.28	12	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.32	13	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.37	14	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.10	15	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Normalized Covariance Matrix

Uncertainty (%)	Correlation															
	Gr.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
9.61	1	1.000	0.844	-0.425	-0.917	-0.669	-0.607	-0.589	-0.586	-0.586	-0.586	-0.589	-0.592	-0.592	-0.592	-0.592
3.37	2	0.844	1.000	0.126	-0.988	-0.964	-0.939	-0.930	-0.929	-0.929	-0.929	-0.931	-0.932	-0.932	-0.932	-0.932
1.00	3	-0.425	0.126	1.000	0.030	-0.388	-0.462	-0.482	-0.484	-0.484	-0.484	-0.480	-0.477	-0.477	-0.477	-0.477
2.81	4	-0.917	-0.988	0.030	1.000	0.910	0.873	0.862	0.860	0.860	0.860	0.862	0.864	0.864	0.864	0.864
5.46	5	-0.669	-0.964	-0.388	0.910	1.000	0.997	0.995	0.994	0.994	0.994	0.995	0.995	0.995	0.995	0.995
6.44	6	-0.607	-0.939	-0.462	0.873	0.997	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.82	7	-0.589	-0.930	-0.482	0.862	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.54	8	-0.586	-0.929	-0.484	0.860	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.83	9	-0.586	-0.929	-0.484	0.860	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.52	10	-0.586	-0.929	-0.484	0.860	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.54	11	-0.589	-0.931	-0.480	0.862	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.38	12	-0.592	-0.932	-0.477	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.42	13	-0.592	-0.932	-0.477	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.47	14	-0.592	-0.932	-0.477	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.20	15	-0.592	-0.932	-0.477	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Multiplication Factor Uncertainties

- Multiplication factor uncertainty were evaluated with four different combinations of covariance matrices and sensitivity coefficients
  - With the normalized covariance matrix, both the unconstrained and constrained sensitivity coefficients yield the same uncertainties
    - *Duplicated use of the normalization condition in sensitivity calculation and covariance matrix generation does not change the result*
  - The uncertainty estimated with un-normalized covariance matrix and constrained sensitivity coefficient is practically same to that obtained with the normalized covariance matrix
    - *Imposition of the fission spectrum normalization condition on sensitivity coefficient calculation is equivalent to renormalizing the covariance matrix of fission spectrum to satisfy the zero-sum constraints*

Sensitivity coefficient	Covariance matrix	
	Un-normalized	Normalized
Unconstrained	0.384	0.301
Constrained	0.300	0.301

Effects of Numerical Precision of Covariance Matrix

- There was a concern about the numerical precision of covariance matrix
  - Need to change ENDF format from single precision to double precision?
- In order to examine the numerical precision effects of the covariance matrix, the multiplication factor uncertainty was recalculated
  - By rounding off the normalized covariance data from five significant digits to three significant digits
- The results suggest that double precision may not be necessary, although further study needs to be done

Sensitivity coefficient	Covariance matrix	
	5 digits	3 digits
Unconstrained	0.30112	0.30120
Constrained	0.30130	0.30131

Conclusions

- The method to renormalize the covariance matrix to satisfy the zero-sum constraint is a congruent transformation of the covariance matrix using the oblique projection operator that maps the normalized fission spectrum space onto itself
  - When the covariance matrix is already normalized, this transformation does not change the covariance matrix
- Imposition of the fission spectrum normalization condition on sensitivity coefficient calculation is equivalent to renormalizing the covariance matrix to satisfy the zero-sum constraints
- Both unconstrained and constrained sensitivity coefficients yield the same response uncertainty when a normalized covariance matrix is used
  - If an un-normalized covariance matrix is used, the constrained sensitivity coefficients yield the correct response uncertainty
- The numerical precision used in covariance matrix normalization appears to be of minor importance, although further study needs to be done