Evaluation and Use of the Prompt Fission Neutron Spectrum and Spectra Covariance Matrices in Criticality and Shielding

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Outline

- Constrained sensitivity method for the calculation of fission spectra sensitivity.

1) Yasunobu Nagaya, Ivan Kodeli, Go Chiba, Makoto Ishikawa, "*Evaluation of sensitivity coefficients of effective multiplication factor with respect to prompt fission neutron spectrum*", Nuclear Instruments and Methods in Physics Research A 603 (2009) 485–490

- Evaluation of PFNS and spectra covariance matrices for ^{235}U, ^{238}U and ^{239}Pu.

2) Ivan Kodeli,, Andrej Trkov, Roberto Capote, Yasunobu Nagaya, Vladimir Maslov, " *Evaluation and use of the prompt fission neutron spectrum and spectra covariance matrices in criticality and shielding*," Nuclear Instruments and Methods in Physics Research A **610** (2009) 540–552

3) **OECD/NEA WPEC Subgroup 26** Final Report, Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations (Feb. 2008) APPENDIX M: I. Kodeli, M.Ishikawa, G. Aliberti, Evaluation of Fission Spectra Uncertainty and their Propagation

Objectives

Investigate:

1. Validation of fission spectrum covariance preparation and processing (analytical and MC)
2. Study practical implications of sensitivity profile normalisation
3. Apply uncertainty analysis to criticality (k_{eff}) and shielding of different reactor systems;
4. Differences between ENDF/B-VII, Watt, Kornilov model spectra, and their consistency with the estimated uncertainties.

Recommendations of WPEC-WG26

Data Formats for Cross Section Covariances in Evaluated Data Files

- ***MF*=31:** covariance of average number of neutrons per fission (ν - MT=452, 455, 456)
- ***MF*=32:** Shape and area of individual resonances
- ***MF*=33:** covariance of neutron cross section
- ***MF*=34:** covariance of angular distribution of secondary neutron (currently MT=2/P_1 only)
- ***MF*=35:** covariance of energy distribution of secondary particles (currently MT=18 only)

No processing available:

- ***MF*=30**: Covariances obtained from parameter covariances and sensitivities
- ***MF*=40**: Covariances for production of radioactive nuclei

Processing available (NJOY-ERRORR and ERRORJ)

Prompt fission neutron spectra

Maxwell distribution

$$\chi(E) = \frac{2\cdot\sqrt{E}}{\sqrt{\pi\cdot T^3}} e^{-E/T}$$

Watt distribution

$$W(E,a,b) = \frac{2}{\sqrt{\pi a^3 b}} \sinh\sqrt{bE} \exp -\left(\frac{ab}{4} + \frac{E}{a}\right)$$

U-235
a=0.988 MeV ± 1.2%
b=2.249/MeV ± 5.9%

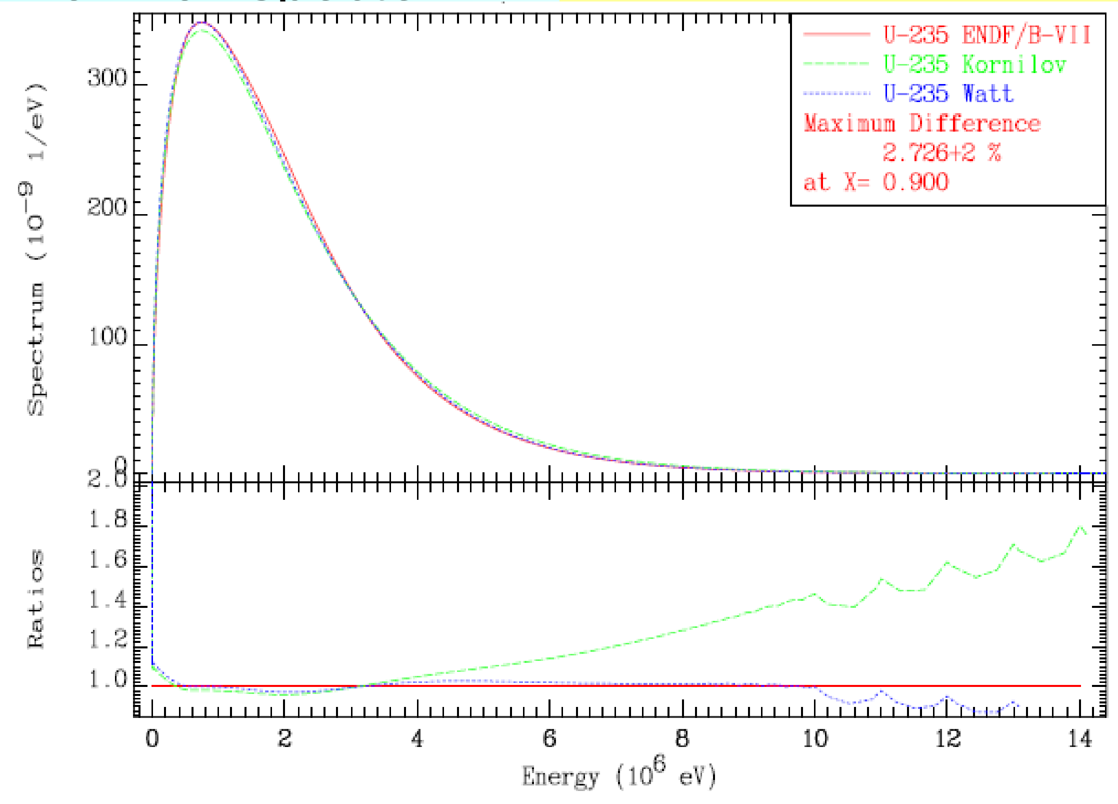
Kornilov specter

$$W(E,r,\alpha) = \frac{W_L(E,T_L,\alpha\varepsilon_L) + W_H(E,T_H,\alpha\varepsilon_H)}{2}$$

U-235

$$r = \frac{T_L}{T_H} = 1.248 \pm 0.031$$

$$\alpha = 0.936 \pm 0.027$$



ENDF/B-VII: Madland-Nix model

Prompt fission neutron spectrum properties

- Fission spectrum is normalised to 1
  sum of bin probabilities equals 1:

$$\sum_g \chi_g = 1$$

- To assure that the perturbed spectrum remains normalised the covariance matrix should comply with the «zero sum» rule: sum of absolute matrix elements in each line and column must be zero:

$$\sum_g \overline{\delta\chi_g \delta\chi_{g'}} = 0$$

- Covariances are given as absolute covariances of the bin probabilities (not average probability distributions)

Normalisation applied to the sensitivity coefficients

- If the matrix does not sattisfy the “zero sum” rule, the ENDF-6 manual suggests the correction formula:

$$\tilde{V}_{i,j} = V_{i,j} - \chi_i \sum_k V_{k,j} - \chi_j \sum_k V_{k,i} + \chi_i \chi_j \sum_{k,k'} V_{k,k'}$$

or in matrix notation: $\tilde{V} = S_\chi^{\,t} \cdot V \cdot S_\chi$ $\quad S^{\chi}_{g,g'} = \delta_{g,g'} - \chi_{g'}$

- Instead of “correcting” the matrices, we can apply the «correction» to the sensitivities :

$$(\Delta R)^2 = S_R^t \cdot \tilde{V} \cdot S_R = S_R^t \cdot \left(S_\chi^{\,t} \cdot V \cdot S_\chi\right) \cdot S_R$$

$$= \left(S_\chi \cdot S_R\right)^t \cdot V \cdot S_\chi \cdot S_R = S_{RN}^t \cdot V \cdot S_{RN}$$

Normalised sensitivities

SAGEP, SUSD3D

Constructing fission spectra covariance matrices– analytic method

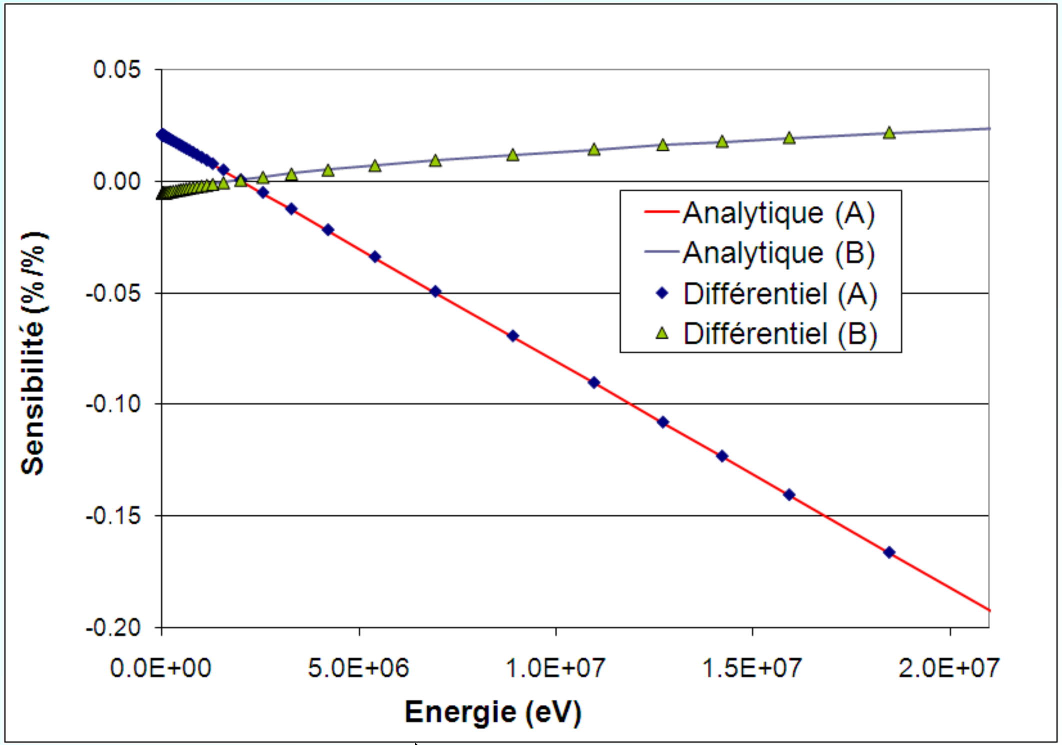
$$M_\chi = S_{ab}^T \cdot M_{ab} \cdot S_{ab}$$

- Covariance matrix of the parameters *a* and *b* of the watt spectrum:

δa/a=1.2%

δb/b=5.9%

$$R = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$$



$$(\Delta R)^2 = S_R^T \cdot \widetilde{V} \cdot S_R = S_R^T \cdot \left(S_\chi{}^T \cdot S_{ab}^T \cdot V_{ab} \cdot S_{ab} \cdot S_\chi\right) \cdot S_R$$

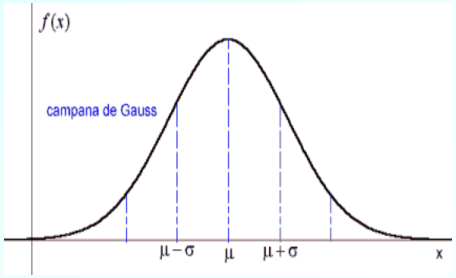
$$= \left(S_{ab} \cdot S_\chi \cdot S_R\right)^T \cdot V_{ab} \cdot \left(S_{ab} \cdot S_\chi \cdot S_R\right) = S_{RN}^T \cdot V_{ab} \cdot S_{RN}$$

ENDF File-30

Constructing fission spectra covariance matrices – Monte Carlo method

- Gaussian probability density distribution of the parameters *a* and *b* (non-correlated):

$$P(a,b) = P(a)\cdot P(b) = \frac{1}{2\pi\cdot\delta a\cdot\delta b}\cdot e^{-\frac{1}{2}\left[\left(\frac{a-\bar{a}}{\delta a}\right)^2+\left(\frac{b-\bar{b}}{\delta b}\right)^2\right]}$$



- Mean: $$\overline{\chi}_g = \sum_i P(a_i,b_i)\chi_g(a_i,b_i) = \frac{1}{n}\sum_{i=1}^{n}\chi_{g,i}$$

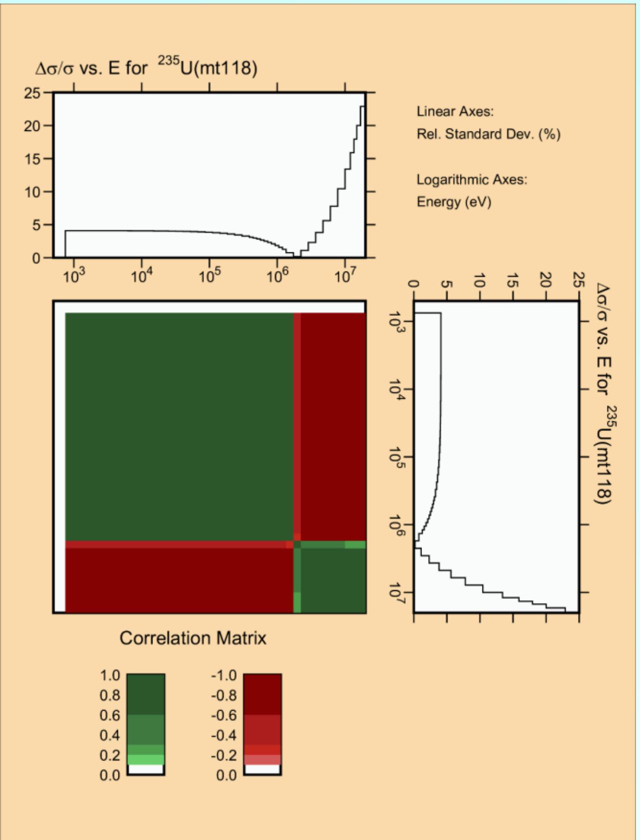
- Covariance: $$\overline{\delta\chi_g\cdot\delta\chi_{g'}} = \sum_{i=1}^{n} P(a_i,b_i)\left(\chi_g(a_i,b_i)-\overline{\chi_g}\right)\left(\chi_{g'}(a_i,b_i)-\overline{\chi_{g'}}\right)$$

$$= \frac{1}{n}\sum_{i=1}^{n}\left(\chi_{g,i}-\overline{\chi_g}\right)\left(\chi_{g',i}-\overline{\chi_{g'}}\right)$$

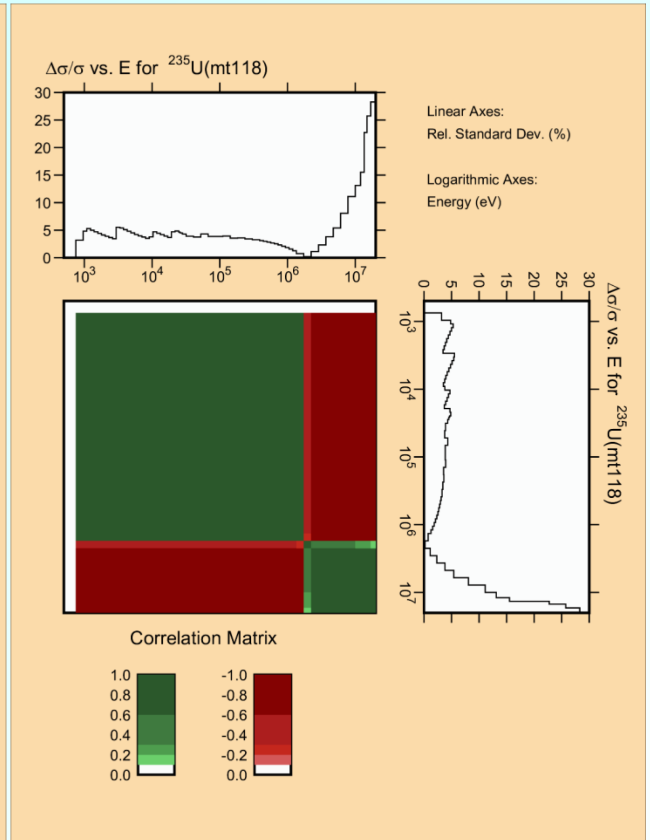
Parameters (r,α) of Kornilov PFNS and parameters (a,b) of Watt model

Parameter	U-235	U-238	Pu-239
$r=T_l/T_h$	1.1215±3.0%	1.248±3.1%	1.1215±3.0%
α	0.905±3.0%	0.880±3.0%	0.823±5.1%
a	0.988±1.2%	0.881±1.2%	0.966±1.2%
b	2.249±5.9%	3.401±5.9%	2.842±5.9%

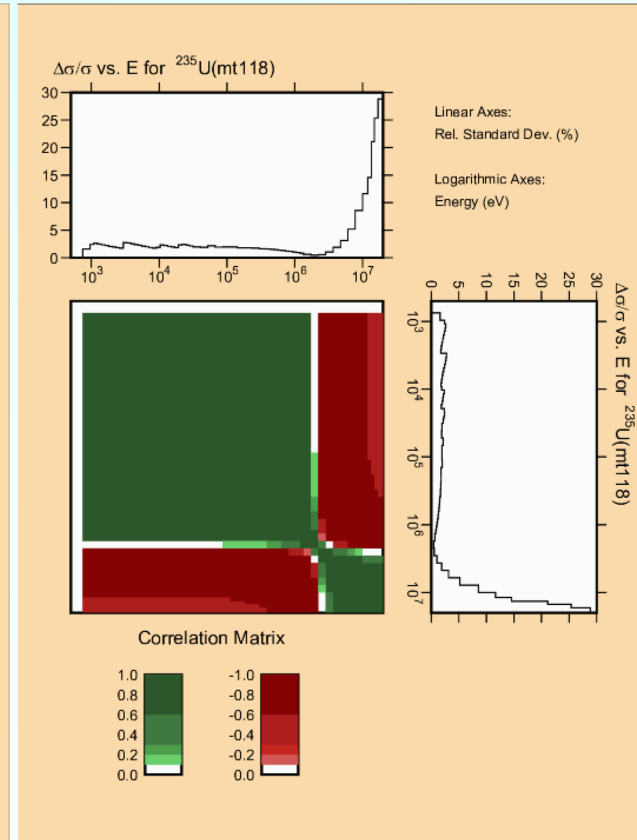
Covariance matrices of U-235 fission spectrum



Analytic-WATT



MC-WATT



MC-Kornilov

VENUS-3 benchmark

Fission averaged detector cross-sections					
Detector	Measured	New Kornilov	Watt	JENDL-3.3	ENDF/B-VII.0
^{27}Al(n,a) [mb]	0.706	0.699 ± 11.1%	0.742 ± 11.1%	0.732 ± 14.1%	0.746
^{58}Ni(n,p) [b]	0.1085	0.1056 ± 3.0%	0.1085 ± 4.0%	0.1072 ± 5.2%	0.1075
^{115}In(n,n') [b]	0.1903	0.1851 ± 1.2%	0.1871 ± 1.7%	0.1883 ± 2.5%	0.1881

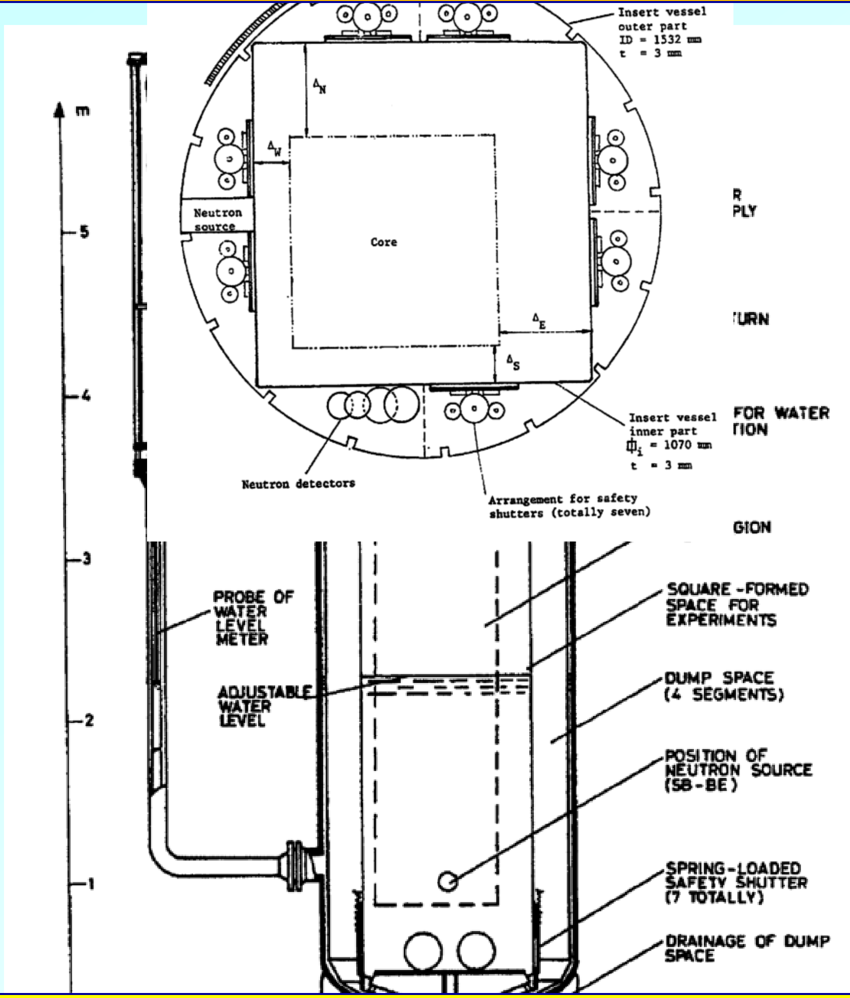
Reaction rates	Uncertainty (%)			RR ratio (New Kornilov/B7)
	New Kornilov	Watt	JENDL-3.3	
^{27}Al(n,a)	11.5	11.5	14.5	0.95
^{58}Ni(n,p)	4.9	5.9	7.6	0.98
^{115}In(n,n')	2.8	3.3	5.2	0.98

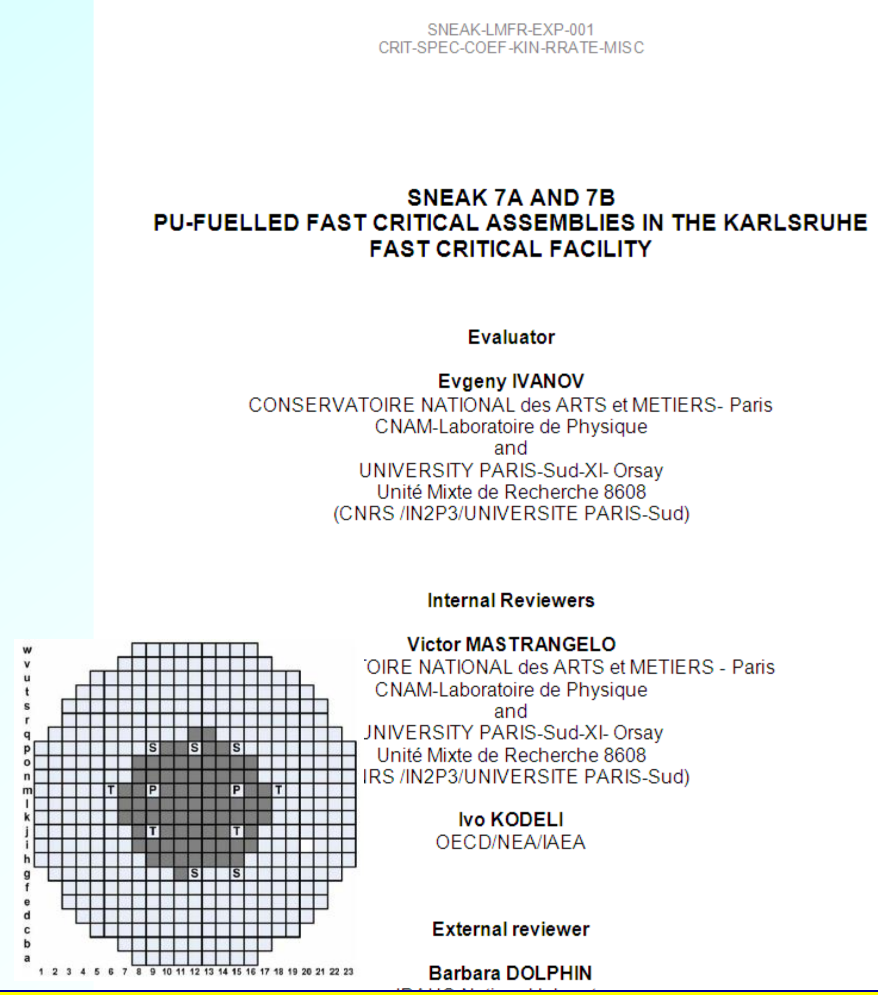
Pressure Vessel Dosimetry

Reaction rate	Uncertainty (%)			RR ratio (New Kornilov/B7)
	New Kornilov	Watt	JENDL-3.3	
^{56}Fe(n,p)	6.0	6.8	8.7	0.989
^{58}Ni(n,p)	5.7	6.5	8.1	0.986
^{63}Cu(n,)	11.0	10.9	13.9	0.981
^{237}Np(n,f)	2.8	3.7	5.0	0.987
^{238}U(n,f)	3.7	4.6	6.0	0.987

IRPhE-International Reactor Physics Experiments Database (OCDE/AEN)

KRITZ-2 –thermal benchmarks 6 critical configurations with UO2 and MOX fuel.	SNEAK-7 – fast benchmarks 2 configurations MOX





SNEAK-LMFR-EXP-001
CRIT-SPEC-COEF-KIN-RRATE-MISC

SNEAK 7A AND 7B
PU-FUELLED FAST CRITICAL ASSEMBLIES IN THE KARLSRUHE FAST CRITICAL FACILITY

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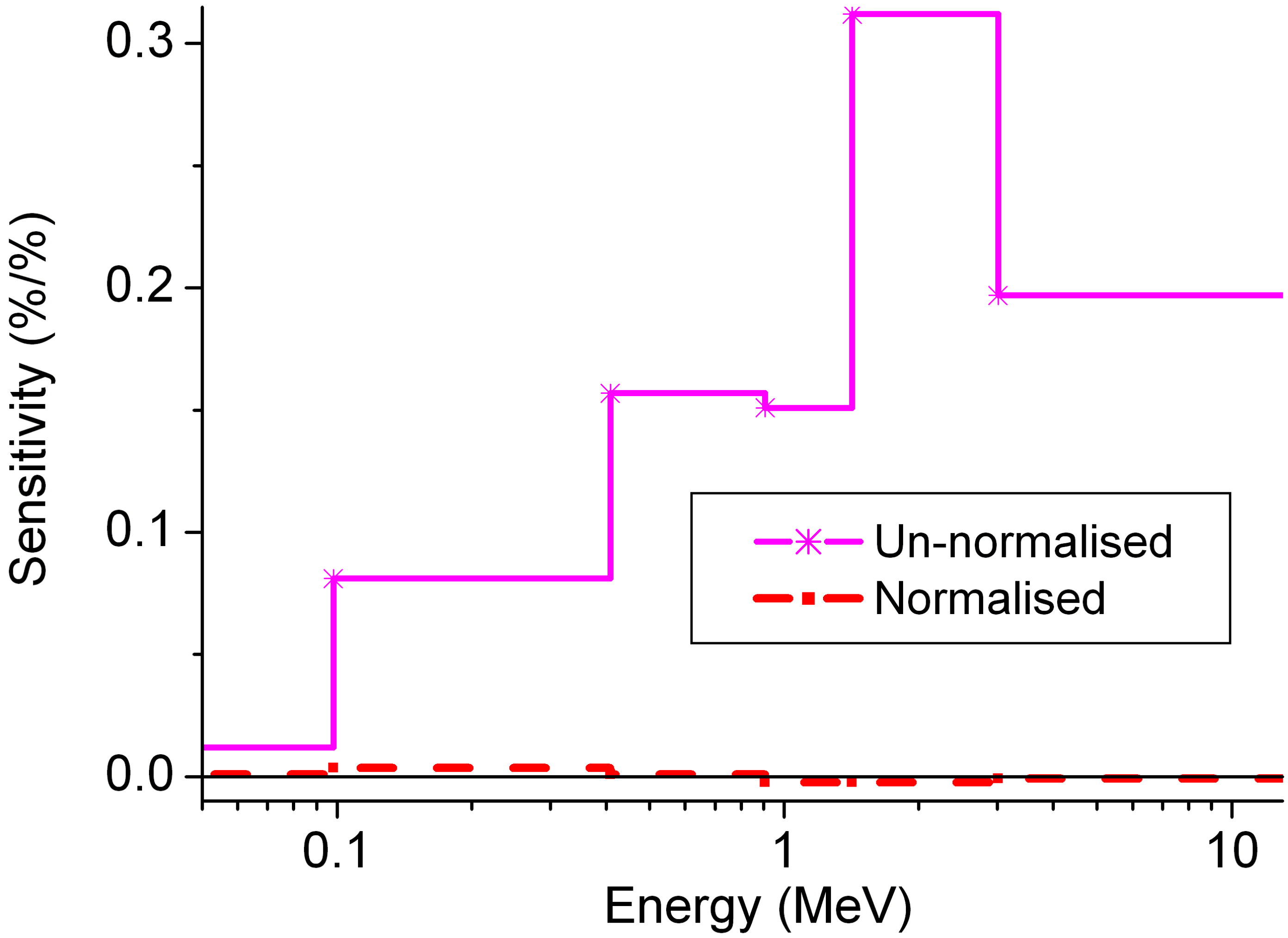
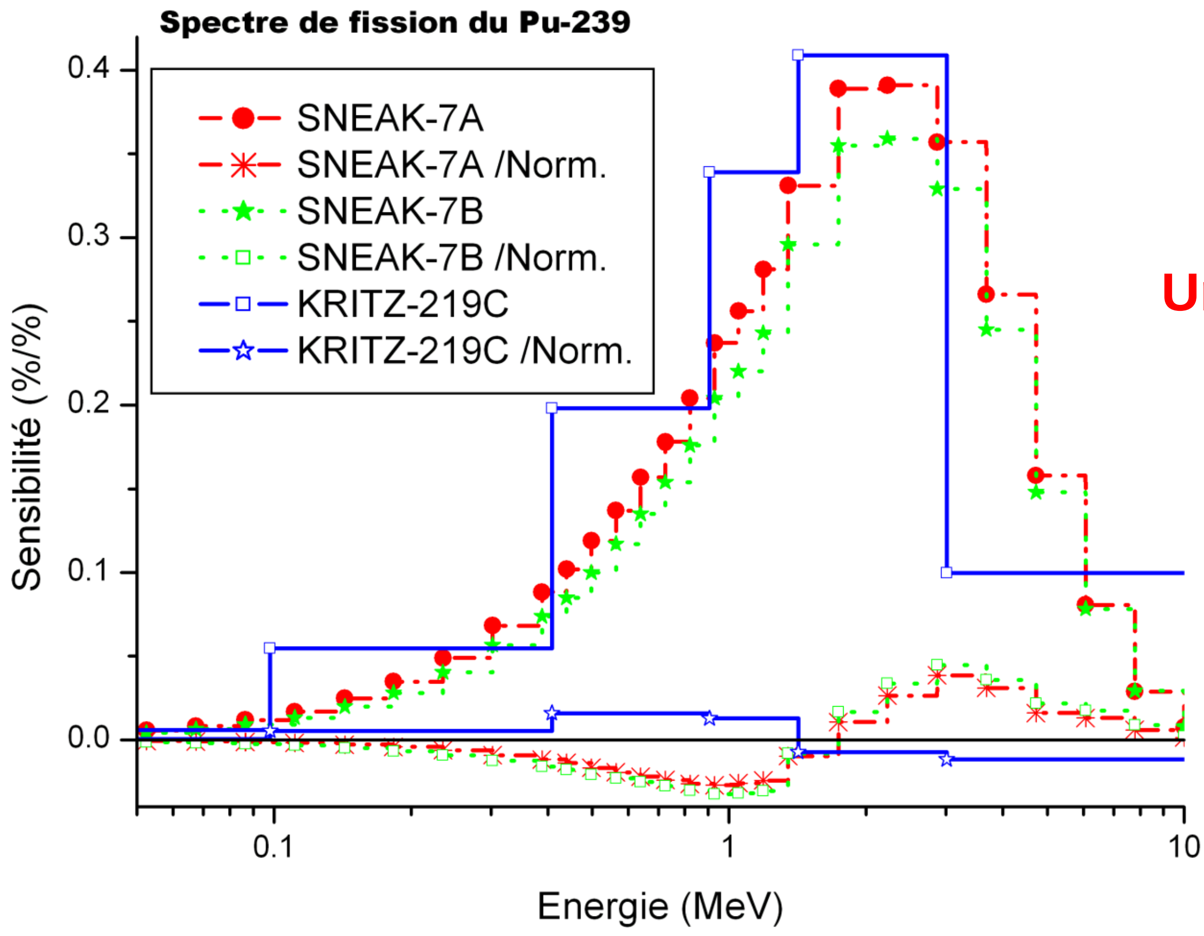
Analysis based on déterministic transport (TWODANT, THREEDANT) and cross section sensitivity and uncertainty code (SUSD3D)

Normalised and un-normalised sensitivities

Sensitivity to ^{235}U fission spectrum (KRITZ-201C benchmark)



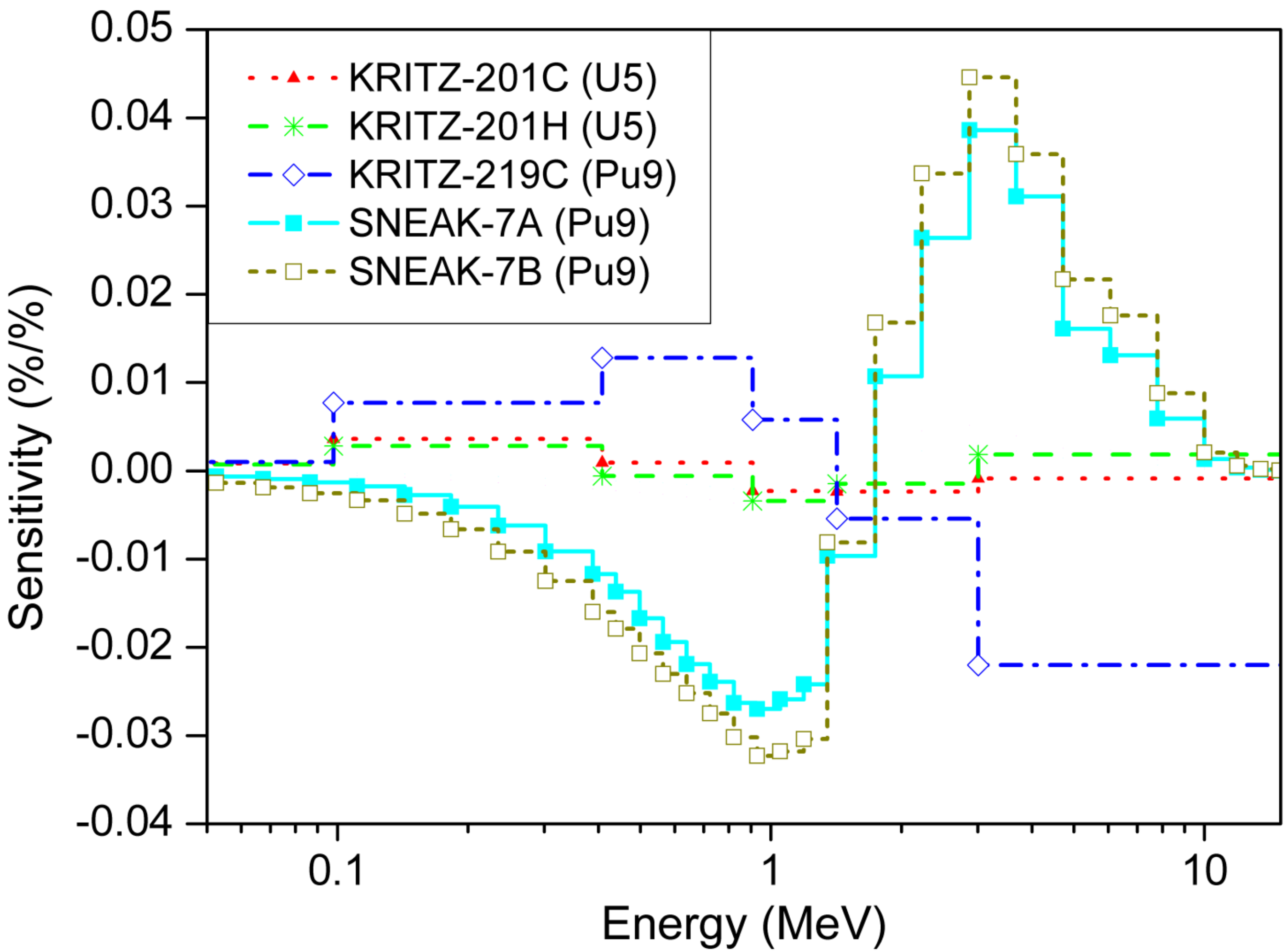
Normalised and un-normalised sensitivities



Un-normalised

Normalised

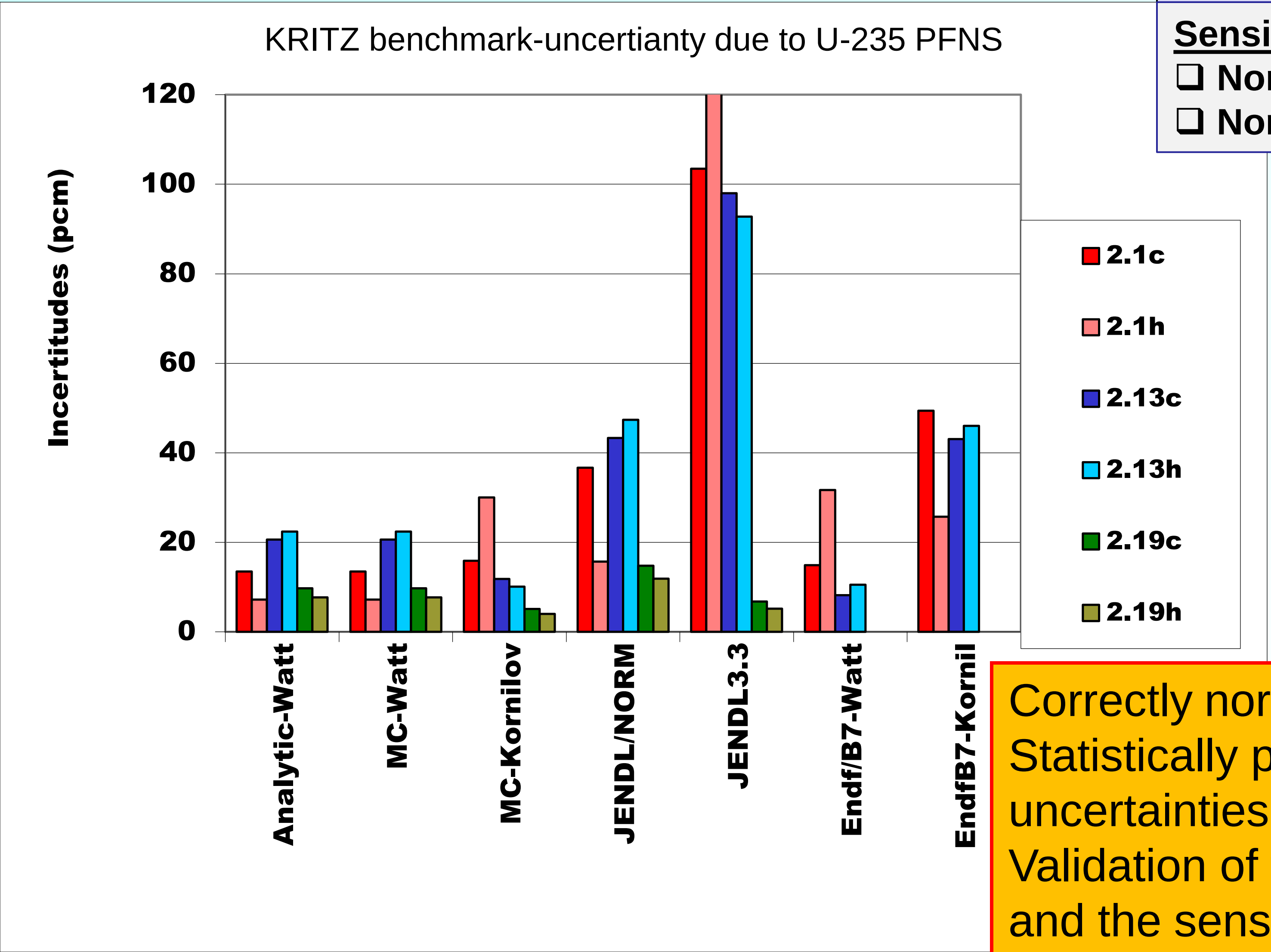
Normalised sensitivity TO PFNS



Uncertainty in *k-eff* (pcm) due to **U-235** fission spectra uncertainty (KRITZ)

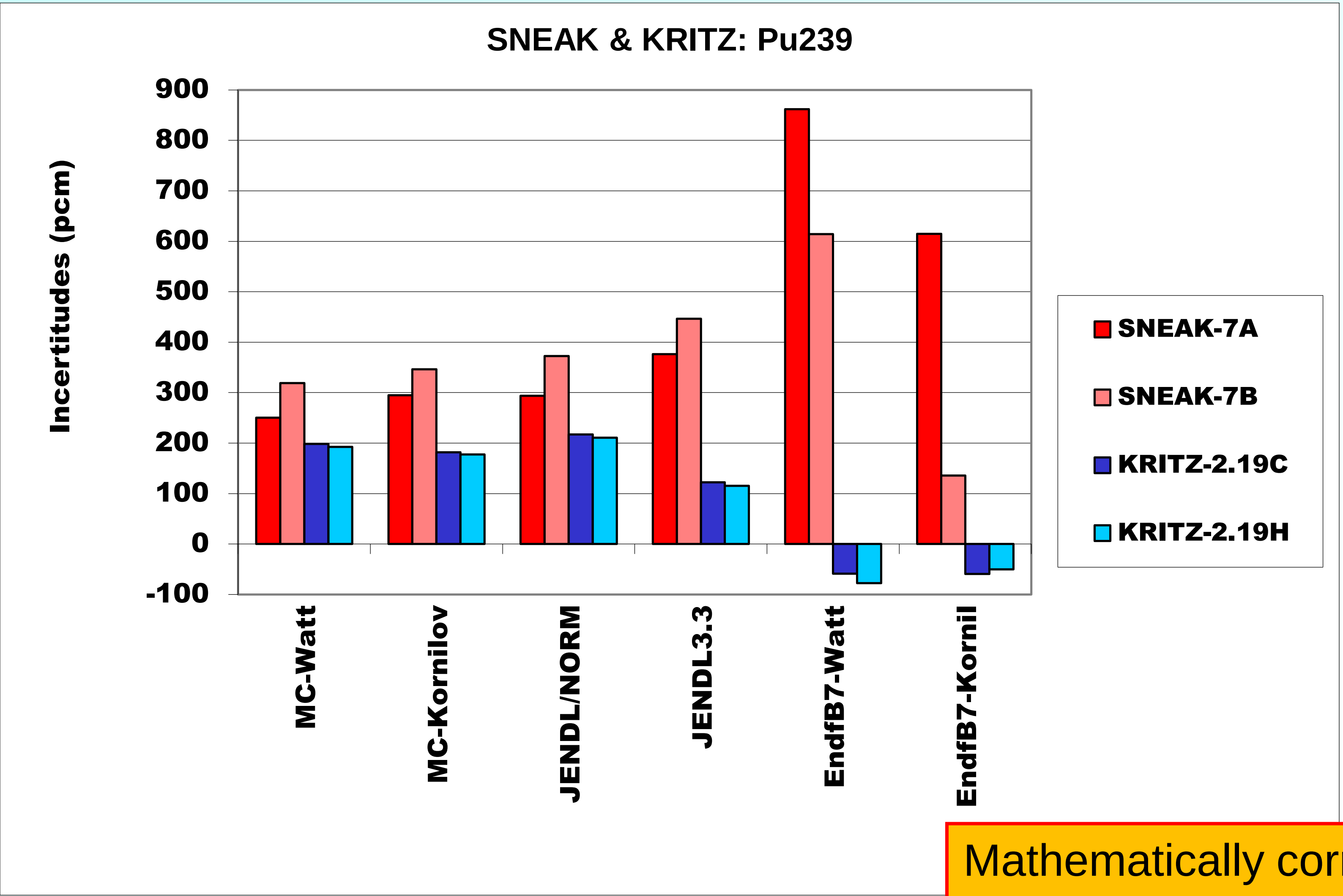
Covariance matrices
- ❑ ***Analytic-Watt***
- ❑ ***MC-Watt***
- ❑ ***MC-Kornilov***
- ❑ ***JENDL3.3***

Sensitivities
- ❑ **Normalised**
- ❑ **Non-normalised**



Correctly normalised matrices; Statistically probable uncertainties ; Validation of the MC method and the sensitivity method.

Uncertainty in k-eff (pcm) due to **Pu-239** fission spectra uncertainty (SNEAK-80g and KRITZ-18g)



Mathematically correct matrices
Statistically plausible

Conclusions

- **MC method** was used to produce covariances for **^{235}U, ^{238}U** & **^{239}Pu fission spectra** based on the Watt and Kornilov models. Spectra were validated against an analytical approach restricted to linear approximation.
- MC method can be applied with confidence to non-linear models, such as optical model.
- **"Normalised" sensitivity method** (discussed during WPEC-SG26) was implemented in SUSD3D. Incorrectly normalised matrices can be detected comparing the uncertainties based on "normalised" and "un-normalised" sensitivities.
- "Normalised" sensitivity method and new covariance matrices were **tested** on sets of thermal and fast critical experiments.
- Uncertainty in *k-eff* due to the fission spectra uncertainties are ~10 - 30 pcm for thermal and **~200 – 300 pcm for fast systems.**
- Differences due to different spectra are consistent with the uncertainties.
- **Difefrences between thermal and fast PFNS uncertainties (fast<th?).**