

# Covariances of prompt fission neutron spectra

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# Objectives

## Investigate:

1. Validation of fission spectrum covariance preparation and processing (analytical and MC)
2. Effects of different spectra on criticality ( $k_{\text{eff}}$ ) (ENDF/B-VII, Watt, Kornilov model)
3. Consistency of the uncertainties in  $k_{\text{eff}}$  calculated from fission spectrum covariances

# Data Formats for Cross Section Covariances in Evaluated Data Files

- **MF=31**: covariance of average number of neutrons per fission ( $\nu$  - 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<sub>1</sub> 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-ERROR and ERRORJ)***

# Prompt fission neutron spectrum models

Maxwell distribution

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

U-235

Watt distribution

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

$a = 0.988 \text{ MeV} \pm 1.2\%$   
 $b = 2.249/\text{MeV} \pm 5.9\%$

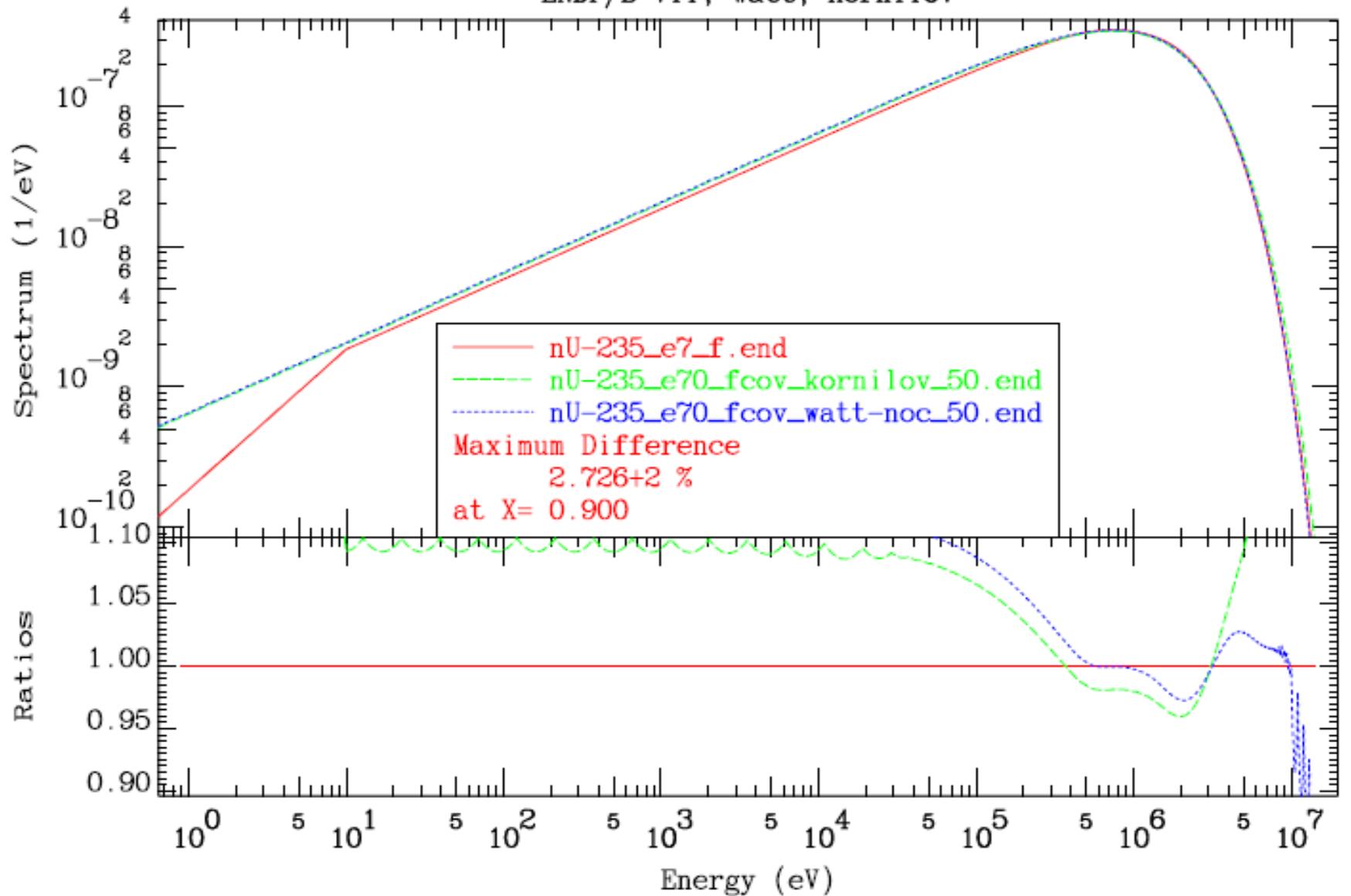
Kornilov spectrum

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

$$W(E, T, \varepsilon) = \frac{1}{\sqrt{\pi T \varepsilon}} \sinh \left[ \frac{2\sqrt{\varepsilon E}}{T} \right] \exp \left[ -\frac{E + \varepsilon}{T} \right]$$

$r = \frac{T_L}{T_H} = 1.248 \pm 0.031$   
 $\alpha = 0.936 \pm 0.027$

Fission Spectrum Comparison  
ENDF/B-VII, Watt, Kornilov



# Prompt fission neutron spectrum properties

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

$$\sum_g \chi_g = 1$$

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

- 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:

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

# Normalisation applied to the sensitivity coefficients

- If the matrix does not satisfy 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:  $\tilde{V} = S_{\chi}^T \cdot V \cdot S_{\chi}$       $S_{g,g'}^{\chi} = \delta_{g,g'} - \chi_{g'}$

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

$$\begin{aligned} (\Delta R)^2 &= S_R^T \cdot \tilde{V} \cdot S_R = S_R^T \cdot (S_{\chi}^T \cdot V \cdot S_{\chi}) \cdot S_R \\ &= (S_{\chi} \cdot S_R)^T \cdot V \cdot S_{\chi} \cdot S_R = S_{RN}^T \cdot V \cdot S_{RN} \end{aligned}$$

Normalised sensitivities

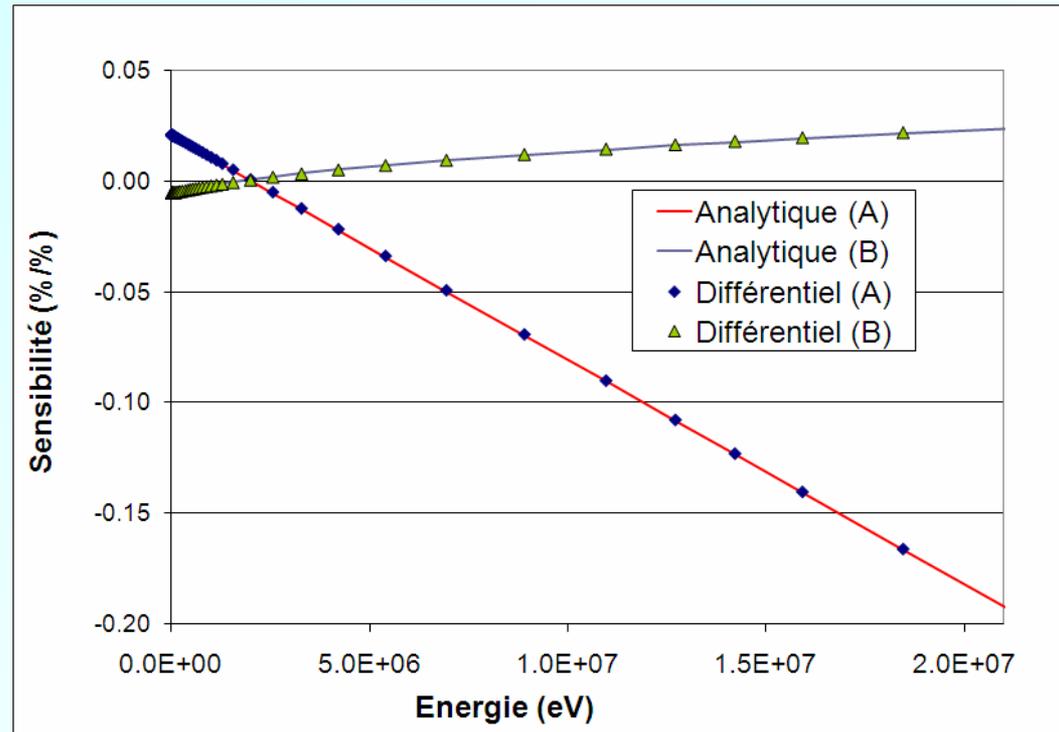
# Constructing fission spectra covariance matrices– **analytic method**

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

□ Covariance matrix of the parameters  $a$  and  $b$  of the watt spectrum:

$$\begin{aligned} \delta a/a &= 1.2\% \\ \delta b/b &= 5.9\% \end{aligned} \quad R = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$$

$$\begin{aligned} (\Delta R)^2 &= S_R^T \cdot \tilde{V} \cdot S_R = S_R^T \cdot (S_{\chi}^T \cdot S_{ab}^T \cdot V_{ab} \cdot S_{ab} \cdot S_{\chi}) \cdot S_R \\ &= (S_{ab} \cdot S_{\chi} \cdot S_R)^T \cdot V_{ab} \cdot (S_{ab} \cdot S_{\chi} \cdot S_R) = S_{RN}^T \cdot V_{ab} \cdot S_{RN} \end{aligned}$$

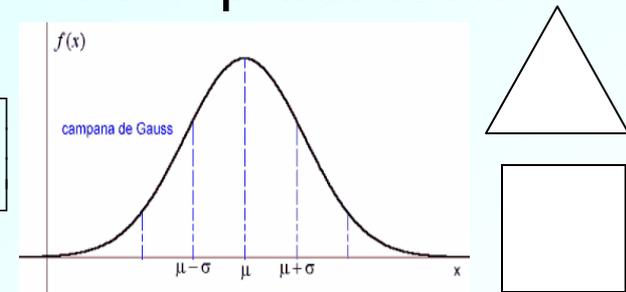


**File-30**

# 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:

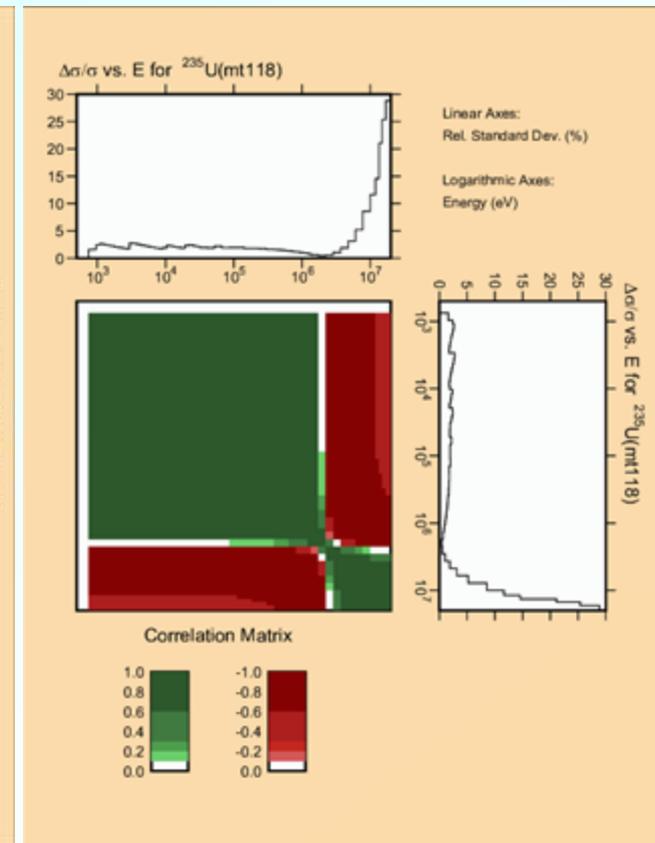
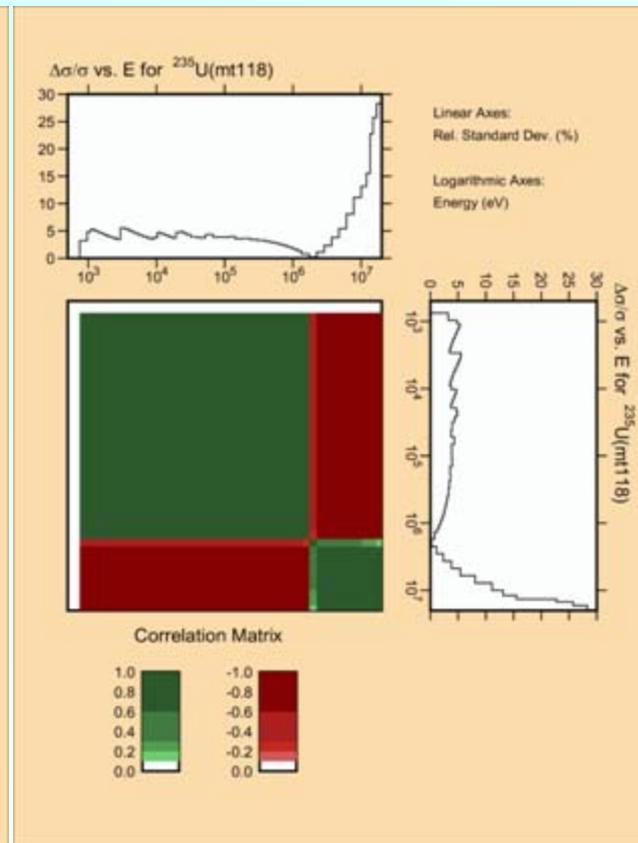
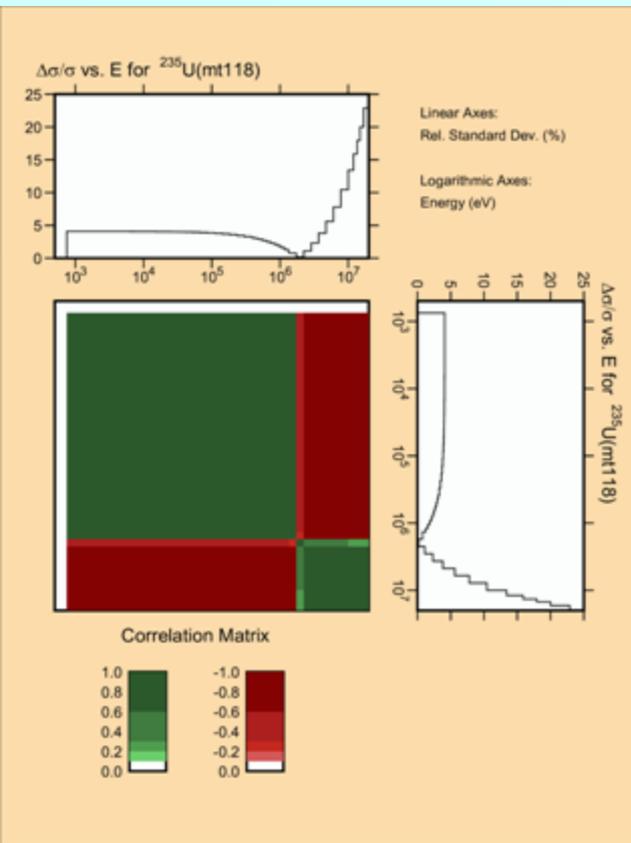
$$\bar{\chi}_g = \sum_i P(a_i, b_i) \chi_g(a_i, b_i) = \frac{1}{n} \sum_{i=1}^n \chi_{g,i}$$

- Covariance:

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

$$= \frac{1}{n} \sum_{i=1}^n \left( \chi_{g,i} - \bar{\chi}_g \right) \left( \chi_{g',i} - \bar{\chi}_{g'} \right)$$

# Covariance matrices of U-235 fission spectrum



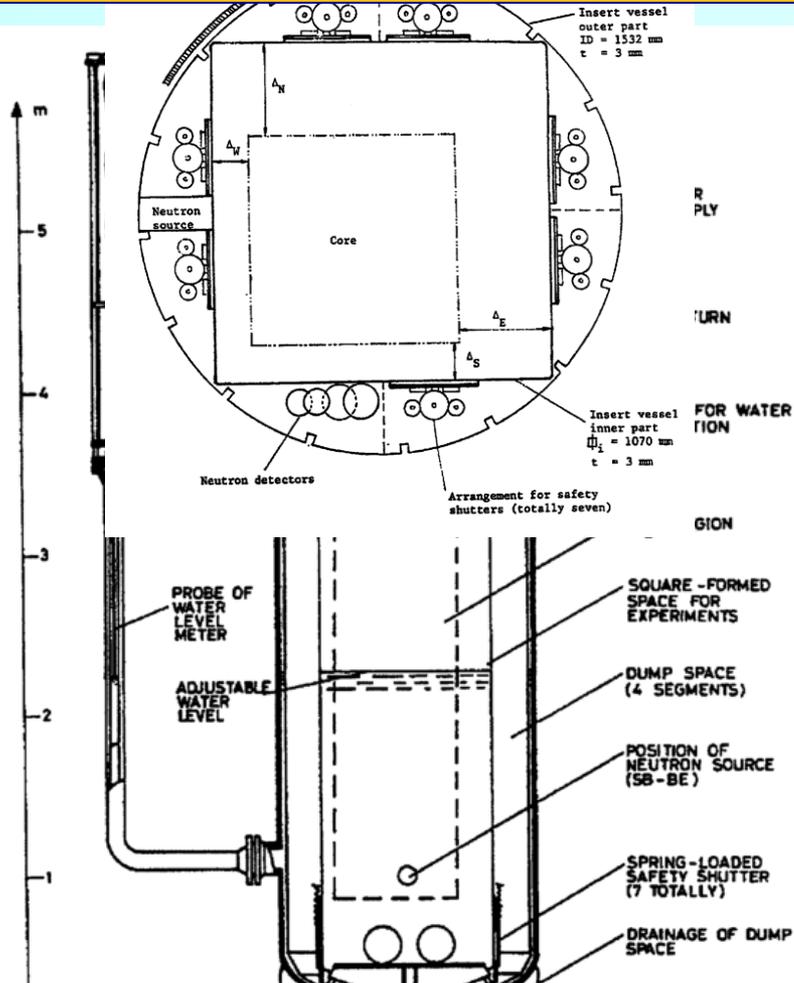
**Analytical-WATT**

**MC-WATT**

**MC-Kornilov**

## KRITZ-2 –thermal benchmarks 6 critical configurations with UO<sub>2</sub> 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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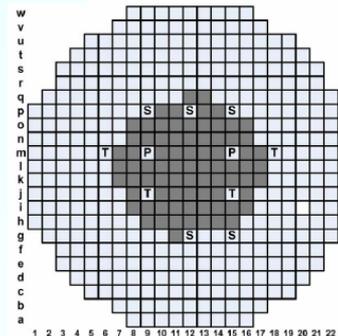
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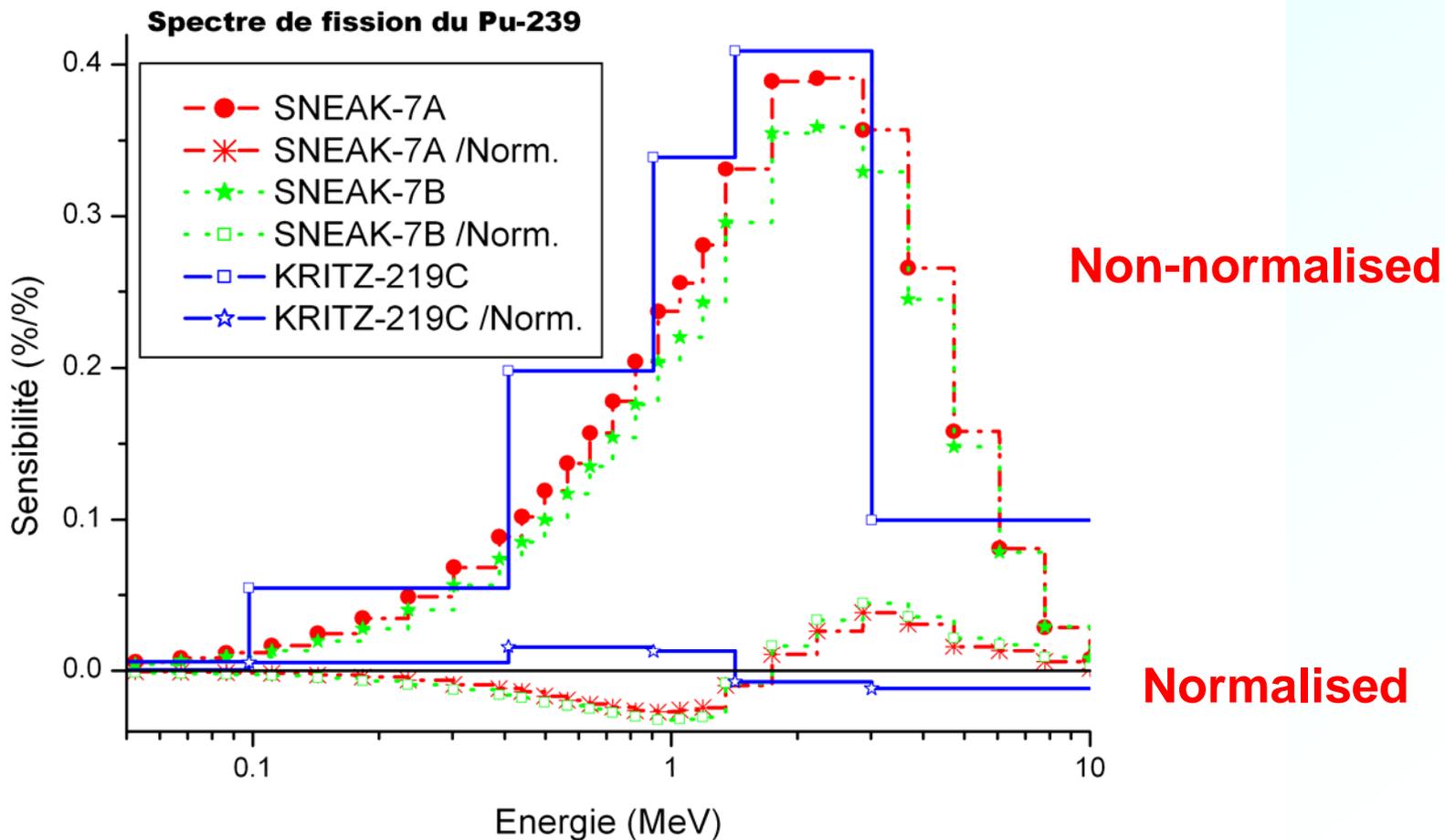
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Analysis based on deterministic transport (TWODANT, THREEDANT) and cross section sensitivity and uncertainty code (SUSD3D)

# Normalised and non-normalised sensitivities



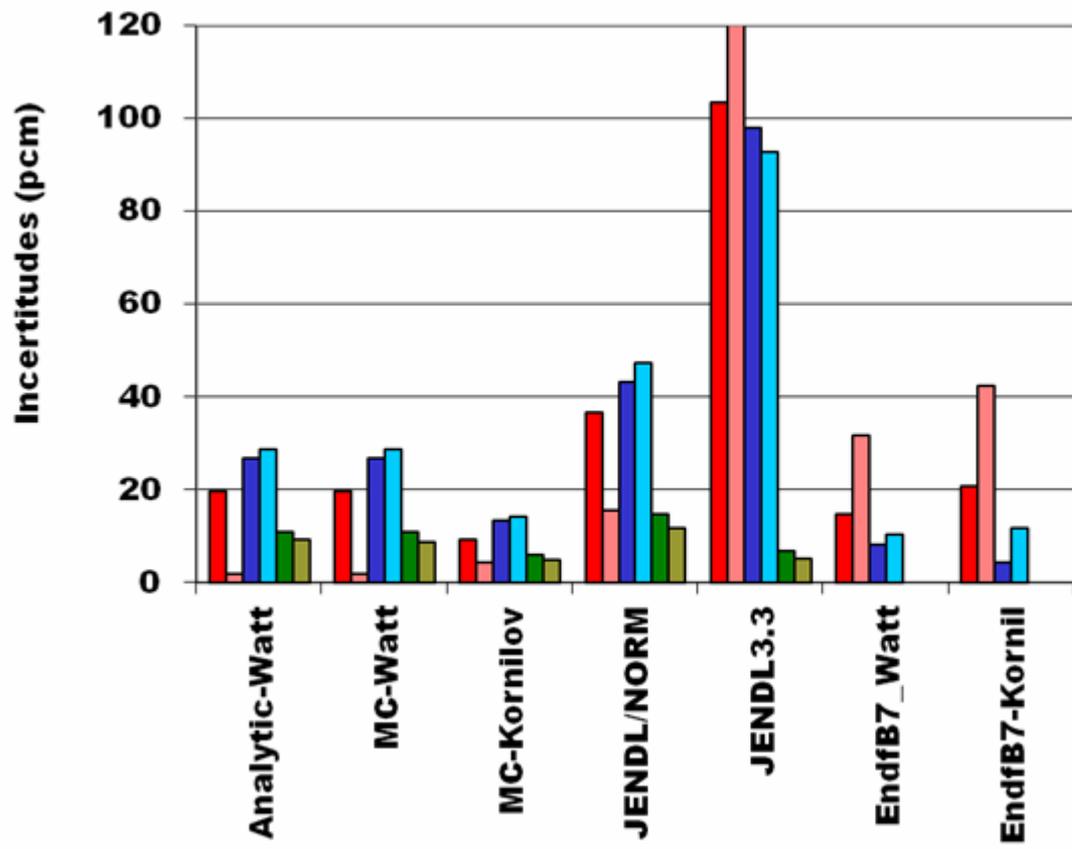
# Differences in k-eff (pcm) due to different fission spectra (relative to ENDF/B-VII)

	$\Delta k_{\text{eff}}$ [pcm]							
	<b>KRITZ</b>						<b>SNEAK</b>	
	<b>2.1c</b>	<b>2.1h</b>	<b>2.13c</b>	<b>2.13h</b>	<b>2.19c</b>	<b>2.19h</b>	<b>7A</b>	<b>7B</b>
Watt	14.9 <sup>a</sup>	31.7	8.2	10.5	-59.0	-77.8	861.7	614.0
Kornilov	20.8	42.3	4.5	11.8	-78.1	-64.1	59.0	171.6

# 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

KRITZ (U-235)

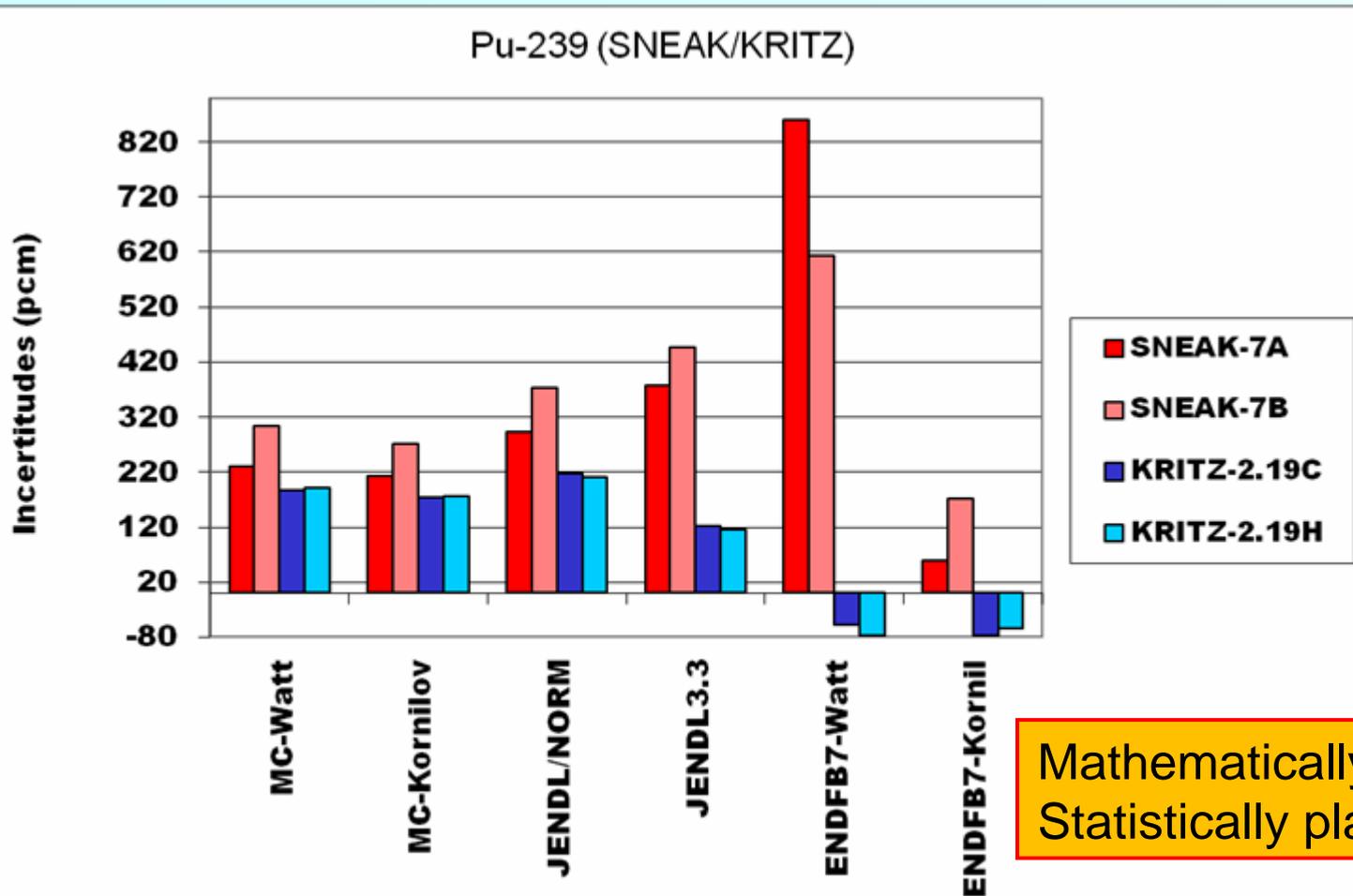


## Kritz-2

- 2.1c (3D)
- 2.1h (2D)
- 2.13c (3D)
- 2.13h (2D)
- 2.19c (3D)
- 2.19h (2D)

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)



# Conclusions

- **MC method** was used to produce covariances for  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  **fission spectra** based on Watt and Kornilov models ( $E < 7\text{MeV}$ ).
- Spectra were **validated** against analytical approach (restricted to linear approximation).
- New “**normalised**” **sensitivity method** (discussed during WPEC-SG26) was implemented in SUS3D.
- “Normalised” sensitivity method and new covariance matrices were **tested** on sets of thermal and fast critical experiments.
- **Incorrectly normalised matrices** give much higher uncertainties.
- Uncertainty in  $k\text{-eff}$  due to the fission spectra uncertainties are  $\sim 10\text{-}30\text{ pcm}$  for thermal and  **$\sim 200 - 300\text{ pcm}$  for fast systems.**
- Differences due to different spectra are consistent with the uncertainties.