Covariance Matrix Evaluation for Independent Fission Yields

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WPEC SG-37 Meeting

May 12, 2014, NEA, Paris

Scope of the work

Main goal

- To produce reliable covariance information on fission yields evaluated in JEFF 3.1.1 .

How

- Development of fission yields models based on free parameters able to reproduce JEFF 3.1.1.
- Bayesian method to generate variance/covariance matrices.

- At this stage only independent fission yields (IFY) have been considered.
- IFY are related to secondary fission fragments, after prompt neutron emission.
- ^{235}U(n_{th}, f) and ^{239}Pu(n_{th}, f) have been used as test fission reactions

Computational Environment

CONRAD (COde for Nuclear Reaction Analysis and Data assimilation), developed at CEA (Cadarache)

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Post-neutron mass fission yield

$$Y_{POST}(140) = Y_{PRE}(140) \cdot p_{140}(0) + Y_{PRE}(141) \cdot p_{141}(1) + Y_{PRE}(142) \cdot p_{142}(2) + \cdots \quad (1)$$

$$Y_{POST}(A) = \sum_{\nu_i=0}^{\infty} Y_{PRE}(A+\nu_i) \cdot p_{A+\nu_i}(\nu_i) \quad (2)$$

- $\mathbf{Y_{POST}(A)}$: Yield for a secondary fission fragment of mass number A.
- $\mathbf{Y_{PRE}(A+\nu_i)}$: Yield for a primary fission fragment of mass $A+\nu_i$ who can contribute to the post-neutron yield $Y_{POST}(A)$ emitting ν_i prompt neutrons.
- $\mathbf{p_{A+\nu_i}(\nu_i)}$: Probability to emit ν_i prompt neutrons for a primary fission fragment of mass $A+\nu_i$.

Pre-neutron mass fission yields

$$Y_{POST}(A) = \sum_{\nu_i=0}^{\infty} \underbrace{Y_{PRE}(A+\nu_i)}_{\text{pre-neutron}} \cdot p_{A+\nu_i}(\nu_i) \quad (3)$$

- $\mathbf{Y_{POST}(A)}$: Yield for a secondary fission fragment of mass number A.
- $\mathbf{Y_{PRE}(A+\nu_i)}$: Yield for a primary fission fragment of mass $A+\nu_i$ who can contribute to the post-neutron yield $Y_{POST}(A)$ emitting ν_i prompt neutrons.
- $\mathbf{p_{A+\nu_i}(\nu_i)}$: Probability to emit ν_i prompt neutrons for a primary fission fragment of mass $A+\nu_i$.

The Brosa model

According to the Brosa model, the pre-neutron distribution for actinides can be described by 5 Gaussians, which correspond to 3 fission modes:

- **Super Long** → Symmetric pre-scission shape (one Gaussian for the symmetric region).
- **Standard I** → Asymmetric pre-scission shape (two Gaussians located symmetrically for light and heavy fragments).
- **Standard II** → Asymmetric pre-scission shape (two Gaussians located symmetrically for light and heavy fragments).

$$Y_{PRE}(A) = \sum_c P_c Y_c(A), \quad c = SL, SI, SII \tag{4}$$

$$Y_c(A) = \frac{1}{\sqrt{2\pi\sigma_c^2}} \left[exp(-\frac{(A_{PRE} - A_c)^2}{2\sigma_c^2}) + exp(-\frac{(A_{PRE} - A_f + A_c)^2}{2\sigma_c^2}) \right] \tag{5}$$

U. Brosa et al., Nuclear Scission, Physics Reports, 197, 4 (1990).

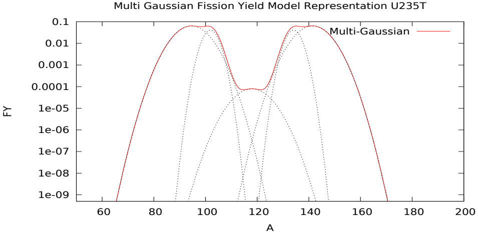
Pre-neutron Parameters

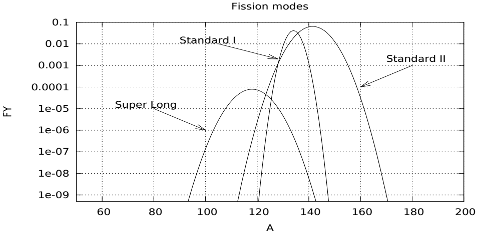
Each fission mode has three parameters:

- **weight**: $\mathbf{P_c}$.
- **deviation**: $\mathbf{D_c} \Rightarrow A_c = \frac{A_f}{2} + D_c$.
- **width**: $\boldsymbol{\sigma_c}$

We do not have 9 free parameters but 7:

- SL is centered in $\frac{A_f}{2}$, where A_f is the compound nucleus mass.
- $\sum_c P_c = 1 \Rightarrow \sum_A Y_{PRE}(A) = 2$.





Prompt neutron emission probability

$$Y_{POST}(A) = \sum_{\nu_i=0}^{\infty} Y_{PRE}(A+\nu_i) \cdot \underbrace{p_{A+\nu_i}(\nu_i)}_{prompt-n \;\; prob.} \tag{6}$$

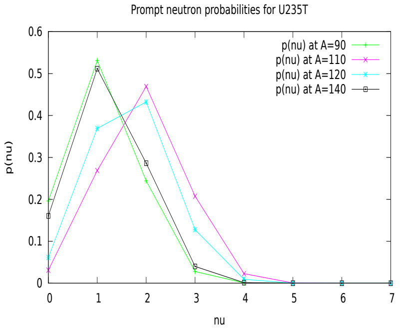
- $\mathbf{Y_{POST}(A)}$: Yield for a secondary fission fragment of mass number A.
- $\mathbf{Y_{PRE}(A+\nu_i)}$: Yield for a primary fission fragment of mass $A+\nu_i$ who contributes to the post-neutron yield $Y_{POST}(A)$ emitting ν_i prompt neutrons.
- $\mathbf{p_{A+\nu_i}(\nu_i)}$: Probability to emit ν_i prompt neutrons for a primary fission fragment of mass $A+\nu_i$.

Prompt neutron emission probability (con't)

We suppose that the probability of the prompt neutron emission for each mass follows a Gaussian law with a constant width.

$$p_A(\nu) = \int_{\nu-0.5}^{\nu+0.5} N \cdot G_{\bar{\nu}(A)}(\nu')d\nu' \quad (7)$$

- $G_{\bar{\nu}(A)}(\nu)$: Gauss distribution
- N: Normalization factor $\Rightarrow \int_0^\infty N \cdot G_{\bar{\nu}(A)}(\nu)d\nu = 1$



Prompt neutron emission probability (con't)

Free Parameters

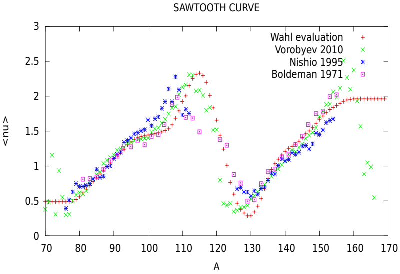
$$p_{A_{PRE}}(\nu_i) = \frac{N}{2} \cdot \left[erf\left(\frac{\nu_i + 0.5 - \bar{\nu}}{\sqrt{2}\sigma}\right) - erf\left(\frac{\nu_i - 0.5 - \bar{\nu}}{\sqrt{2}\sigma}\right)\right]$$

- $\bar{\nu}(A_{PRE})$: central value of the re-normalized Gaussians $N \cdot G_{\bar{\nu}(A_{PRE})}$.
- σ: width of the same function, supposed independent from the mass of the primary fragment.

Prompt neutron emission probability (con't)

Saw-Tooth

- Experimental information about the first momentum of $p_{A_{PRE}}(\nu_i)$ are available $\rightarrow$ saw-tooth curve;
- $\bar{\nu}$ is then related to the average number of prompt neutrons emitted by primary fragments given by the Saw-tooth;
- $\sum_{\nu_i} \nu_i \cdot p_{A_{PRE}}(\nu_i) =< \nu >_{ST}$;
- This equation is iteratively solved in the model.



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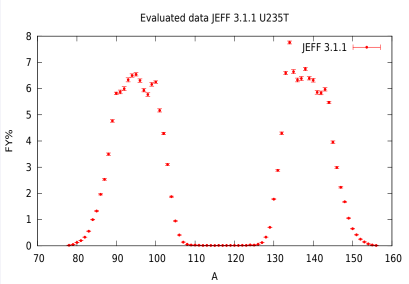
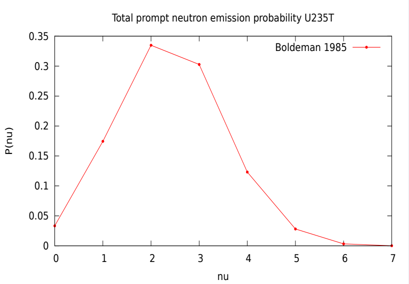
What we want to adjust

- $\mathbf{Y_{PRE}}$: Fission modes parameters, $\mathbf{D_c}$, $\boldsymbol{\sigma_c}$, $\mathbf{P_c}$
- $\mathbf{p_{A_{PRE}}}(\nu_i)$: Prompt-neutron parameters, $\bar{\nu}(A_{PRE})$, σ





$$\bar{\nu}_{tot} = \sum_{0}^{\infty} Y_{PRE}(A) < \nu >_{ST} \quad \bar{\nu}_L = \sum_{0}^{A_f/2} Y_{PRE}(A) < \nu >_{ST} \quad \bar{\nu}_H = \sum_{A_f/2}^{\infty} Y_{PRE}(A) < \nu >_{ST}$$

Generalized Least Square Method

It is based on the Bayes theorem:

$$\vec{p}(\vec{x}|\vec{y},U) = \frac{p(\vec{y}|\vec{x},U)\cdot p(\vec{x}|U)}{\int d\vec{x}\cdot p(\vec{x}|U)\cdot p(\vec{y}|\vec{x},U)} \tag{8}$$

From the Maximum Entropy Theorem we have

$$posterior = p(\vec{x}|\vec{y},U) \propto exp\Big[-\frac{1}{2}(\vec{x}-\vec{x}_{prior})^T \mathbf{M}_x^{prior^{-1}} \cdot (\vec{x}-\vec{x}_{prior}) + (\vec{f}(\vec{x})-\vec{y})^T \mathbf{M}_y^{-1}(\vec{f}(\vec{x})-\vec{y})\Big] \tag{9}$$

$\vec{x}$: parameter vector;
$\vec{y}$: experimental values;
$\vec{f}(\vec{x})$: theoretical model function.

Modeling environment: CONRAD

Using Newton-Raphson to minimize the cost function

$$\vec{x}^{(n)} = \vec{x}^{(n-1)} - \mathbf{M}_x^{(n-1)} \cdot \Big[\mathbf{G}^{(n-1)^T} \mathbf{M}_y^{-1} \cdot \\ (\vec{f}(\vec{x}^{(n-1)}) - \vec{y}) + \mathbf{M}_{\mathbf{x}}^{prior^{-1}} (\vec{x}^{(n-1)} - \vec{x}_{prior}) \Big] \quad (10)$$

$$\mathbf{M}_x^{(n-1)} = \left[\mathbf{M}_x^{prior^{-1}} + \mathbf{G}^{(n-1)^T} \mathbf{M}_y^{-1} \mathbf{G}^{(n-1)} \right]^{-1} \quad (11)$$

CONRAD

COde for **N**uclear **R**eaction **A**nalysis and **D**ata assimilation.
Developed at **CEA** (Cadarache).
The mass fission yield model has been implemented in CONRAD.

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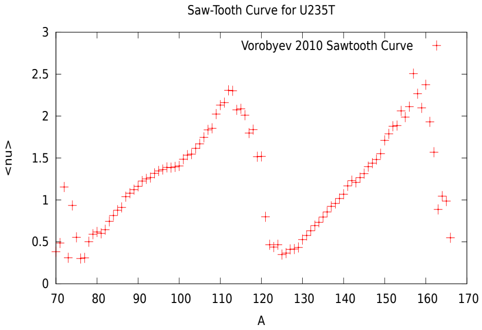
PRIORS

Parameter	Value	Error
Deviation Standard1 (amu)	15.8	0.2
Deviation Standard2 (amu)	23.1	0.2
StdDev Standard1	2.6	0.05
StdDev Standard2	4.95	0.05
StdDev Super Long	5.05	0.0505
Weight Standard1	0.162	0.005
Weight Super Long	0.0012	0.00012

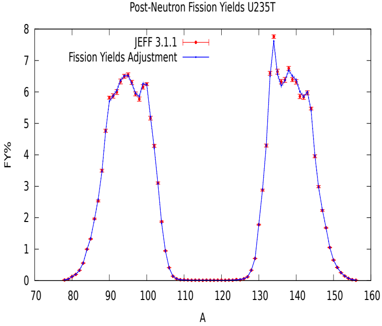
S. Zeynalov, V. Furman, F.-J. Hambsch, 'Investigation of mass-TKE distributions of fission fragments from the ^{235}U(n,f)-reaction in resonances', Proc. of the 13th ISINN Workshop, May 2005, Dubna.

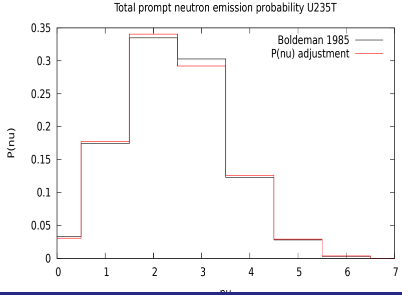


A.S. Vorobyev et al., Investigation of the prompt neutron emission mechanism in low energy fission of ^{235,233}U(n_{th}, f) and ^{252}Cf(sf). EPJ Web Conf., 8, October 2010

Adjusted parameters

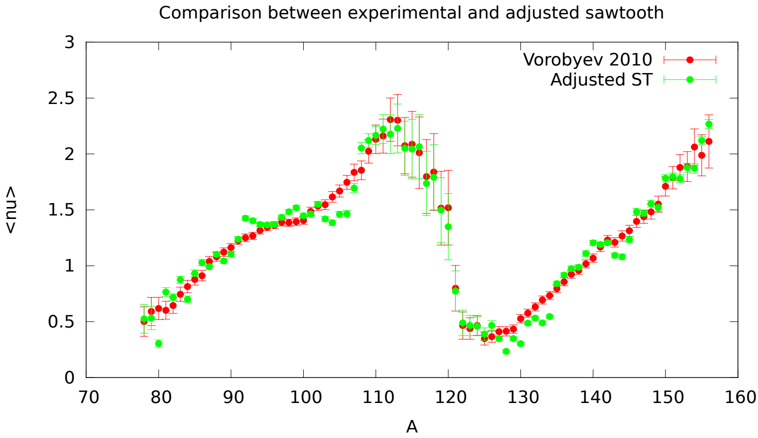
Parameter	Prior	Posterior
Deviation Standard1 (amu)	15.8	16.0088
Deviation Standard2 (amu)	23.1	23.2879
StdDev Standard1	2.6	2.0927
StdDev Standard2	4.95	4.82134
StdDev Super Long	5.05	5.03229
Weight Standard1	0.162	0.211697
Weight Super Long	0.0012	0.00150245





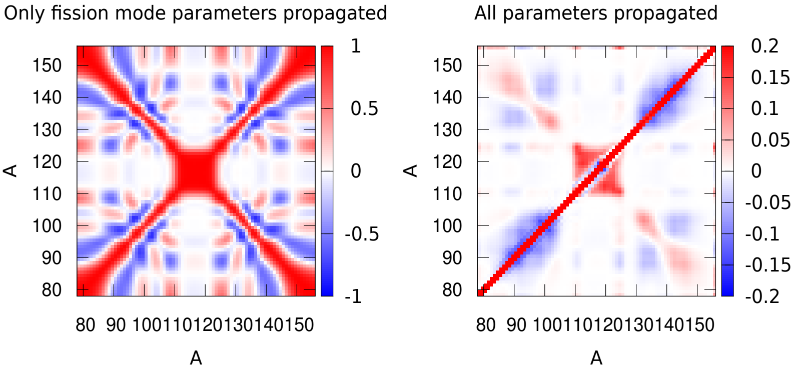
Parameter	Best Estimate
σ prompt-n emission prob.	0.855

Adjusted Saw-Tooth



Correlation matrix for fission yields U235T

After adjustment, statistical errors only

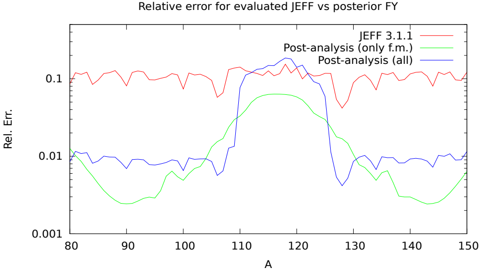


- Correlation matrices have been obtained after adjustment, only statistical uncertainties have been considered.
- Propagating saw-tooth parameters covariances reduces correlations given by the fission modes.
- Without a physical model, the saw-tooth can give correlations only locally.
- The pre-neutron modes give strong correlations between light and heavy fragments. Standard1 and Standard2 are in competition and give anti-correlations.

Relative Errors

JEFF 3.1.1 Relative Error

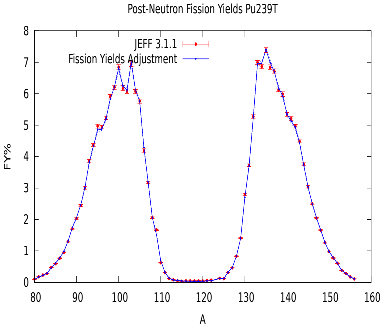
- The uncertainties in JEFF 3.1.1 for mass fission yields are over-estimated.
- They are quadratic sums of the errors on isotopic fission yields.
- In the adjustment procedure we modified the JEFF error to get a better representation on the peaks (99% of the total yield).

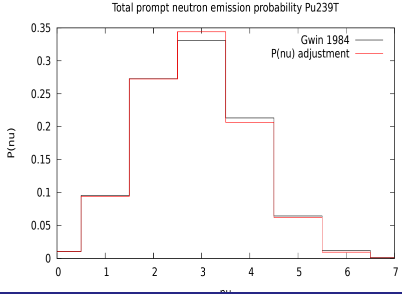


Marginalization is needed to get more reliable relative errors on the final values.

^{239}Pu

Parameter	Prior	Posterior
Deviation Standard1 (amu)	14.97	15.6873
Deviation Standard2 (amu)	20.96	21.6877
StdDev Standard1	3.73	3.24573
StdDev Standard2	6.48	6.30685
StdDev Super Long	15.8	16.0479
Weight Standard1	0.2283	0.370481
Weight Super Long	0.0057	0.00630751

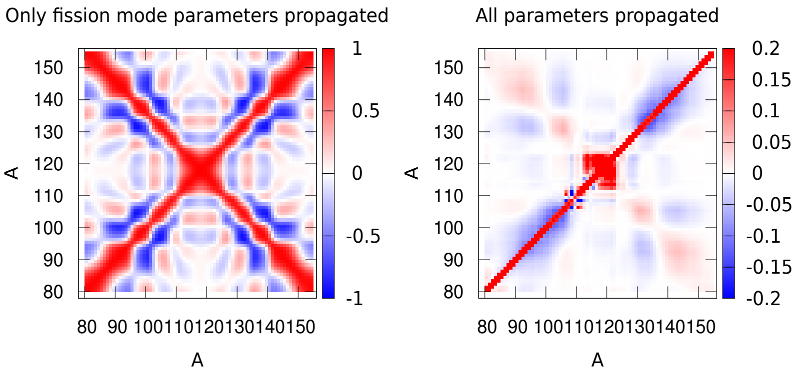




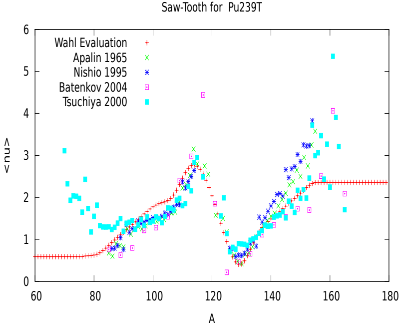
Parameter	Best Estimate
σ prompt-n emission prob.	0.795

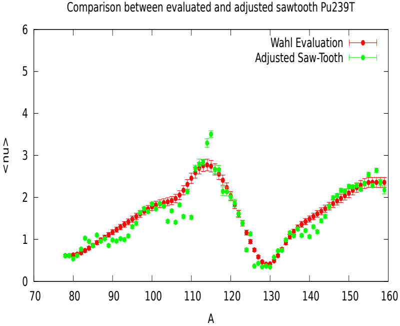
Correlation matrix for fission yields Pu239T

After adjustment, statistical errors only



Adjusted Saw-Tooth Pu239T





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Conclusions

- We have developed a method able to represent faithfully JEFF 3.1.1 evaluations for mass fission yields.
- The adjustment of the parameters for the pre-neutron fission modes and the saw-tooth curve has given acceptable results.
- Preliminary correlation information have been produced for mass fission yields, considering only statistical uncertainties.

Outlook

- Systematic errors must be properly considered in this exercise, using marginalization techniques.
- To get more reliable correlation information and variance-covariance matrices, a model for the saw-tooth curve should be found.
- The same exercise can be done for isotopic and isomeric fission yields adding features in CONRAD.
- Other fissioning systems will be processed in the future.

THANK YOU FOR YOUR ATTENTION