

Decay heat calculations with JEFF-4.0 fission yields and decay data

L. Giot, F. Esposito

Task 4.3.2 Fission yields benchmarking

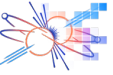
Lausanne, 07/07/2026



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Decay heat calculations



■ Summation method

$$DH(t_c) = f(t_c) = \sum_i^n N_i(t_c) \lambda_i \bar{E}_i$$

N_i : Number of nuclei i at cooling t_c

λ_i : Decay constant

$\bar{E}_i$: Mean decay energy of nucleus i

■ Atomic Densities N_i : solving Bateman's equations

Transport and depletion calculations : reactor model + neutronic code

$$\frac{\partial N_i(t)}{\partial t} = \sum_{j \neq i} (b_{j \rightarrow i} \lambda_j + \langle \sigma_{j \rightarrow i} \phi \rangle) N_j(t) - (\lambda_i + \langle \sigma_i \phi \rangle) N_i(t)$$

production & disappearance per radioactive decays & nuclear reactions

~ 40 000 nuclear data: σ , $\bar{E}$, Branching Ratio, λ , Fission Yields, $\bar{\nu}$

=> Complex calculation (reactor model + depletion)

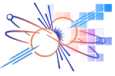
=> Quality of the code but also of the input data !



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Decay heat calculations



■ Summation method

$$DH(t_c) = f(t_c) = \sum_i^n N_i(t_c) \lambda_i \bar{E}_i$$

■ $\bar{E}_i$ usually divided in 3 parts in evaluated libraries(e.g ENDF, JEFF, JENDL) :

$$\bar{E}_{LP} = \bar{E}_{\beta^-} + \bar{E}_{\beta^+} + \bar{E}_{e^-} + \dots \quad \text{Light particles component}$$

$$\bar{E}_{EM} = \bar{E}_{\gamma} + \bar{E}_{x-ray} + \bar{E}_{anni.rad.} + \dots \quad \text{Electromagnetic component}$$

$$\bar{E}_{HP} = \bar{E}_{\alpha} + \bar{E}_{SF} + \bar{E}_p + \bar{E}_n + \dots \quad \text{Heavy particles component}$$

■ $\bar{E}_i$ measurements & Pandemonium effect

Before the 90s, conventional detection techniques: high resolution γ -ray spectroscopy

Excellent resolution but efficiency which strongly decreases with increasing energy

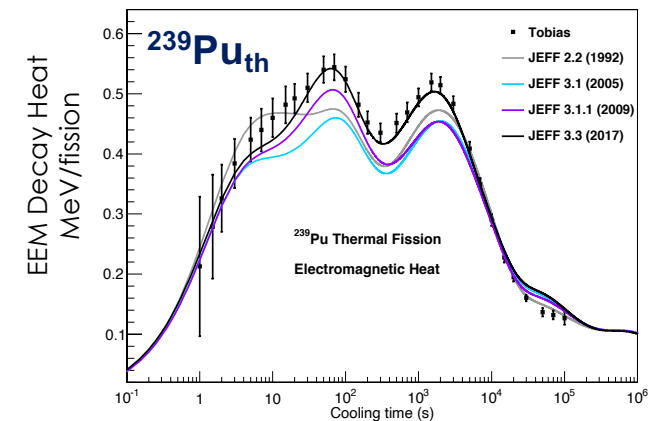
Risk of overlooking the existence of β^- feeding into the high energy nuclear levels of daughter nuclei

Incomplete decay schemes: overestimate $\bar{E}_{\beta^-}$, underestimate $\bar{E}_{\gamma}$

=> Most suitable technique to re-measure key nuclei:

Total Absorption Gamma Spectroscopy using 4π detectors (ex: NaI, LaBr3)

See A. Algora's talk



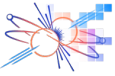
A. L. Nichols et al., EPJ A 59 (2023)



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How/Why to improve FY & Decay data for inventory and DH calculations ?



- From the industry perspective:

validation = calculations (given version of the depletion code + given library) on a set of benchmarks (modeling and/or experimental values), quantification of the differences to get some margins

=> Less feedback on FY and DD new needs or needed improvements wrt XS, $\bar{\nu}$..

=> To be included/more visible in the NEA HPRL list ? => more exchanges ...

ex (from EDF): MOX DH between 10 days and 1 year, contribution of ^{242}Cm

- From the nuclear data perspective:

comparison between experimental values (PIE and DH measurements) and calculations

=> often limited fission pulse cases & assemblies

=> more measurements needed from irradiation experiments

only one measurement set for $^{241}\text{Pu}_{\text{th}}$ & $^{239}\text{Pu}_{\text{fast}}$...

=> The simplest the set-up is, the easiest to disentangle the effects and then to identify the nuclear data to be improved

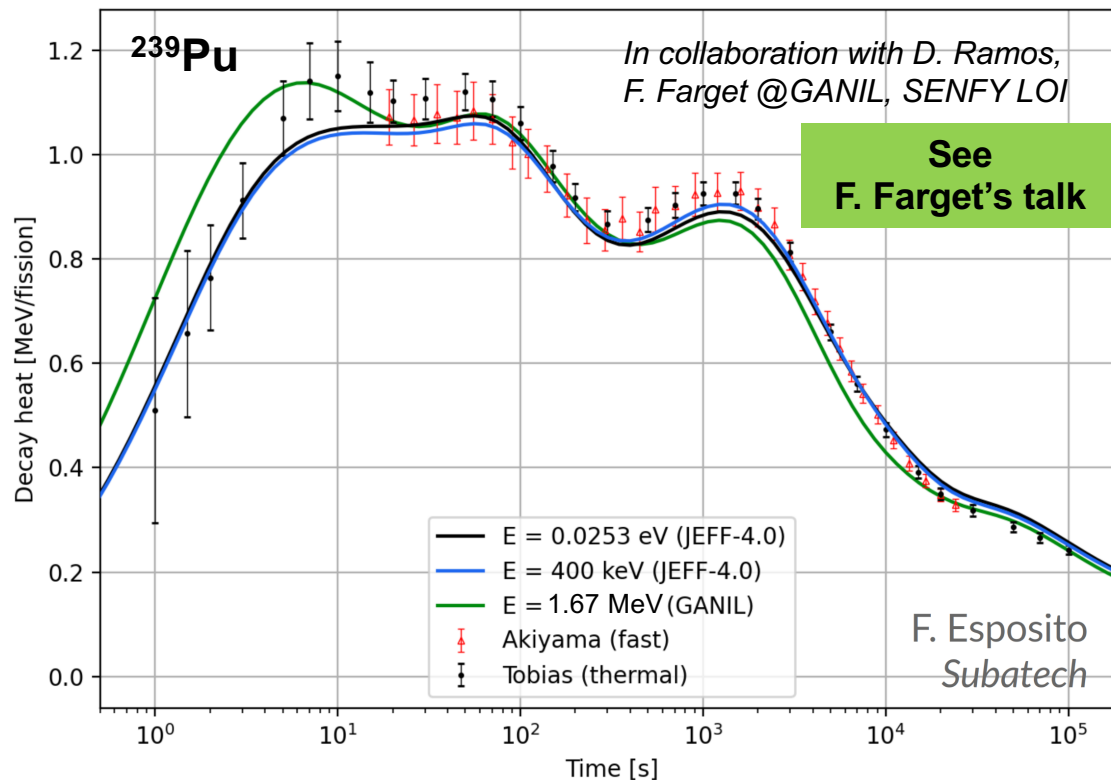
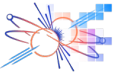
	Nucleus	Measurements	Cooling time	Uncertainty Range %	Year	Authors
Fission induced per thermal neutrons	^{235}U	β, γ	$0.4 - 10^5 \text{ s}$	3.2% - 9.5 % 2.5% - 24.1% 2.5% - 8.6%	1989, 1980, 1997	Dickens, Tobias, Lowell, others
	^{239}Pu	β, γ	$1 - 10^5 \text{ s}$	2.3% - 6.9% 2.7% - 60.9% 2% - 9.9%	1989, 1980, 1997	Dickens, Tobias, Lowell, others
	^{241}Pu	β, γ	$3 - 1.2 \cdot 10^4 \text{ s}$	4% - 11.1%	1980, 1989	Dickens
Fission induced per fast neutrons	^{239}Pu	β, γ	$19 - 2.4 \cdot 10^5 \text{ s}$	2.4% - 5.7%	1982	Akiyama
	^{233}U	β, γ	$19 - 2.4 \cdot 10^5 \text{ s}$	3.2% - 7.5%	1982, 2002	Akiyama, Ohkawachi
	^{235}U	β, γ	$19 - 2.4 \cdot 10^5 \text{ s}$	2.1% - 6.1%	1982	Akiyama
	^{238}U	β, γ	$0.4 - 2.4 \cdot 10^5 \text{ s}$	3.8% - 20% 1.8% - 5.3%	1997, 1998	Akiyama, Lowell
	^{232}Th	γ	$19 - 2.4 \cdot 10^5 \text{ s}$	3.7% - 9.2%	1997	Akiyama
	^{237}Np	γ	$264 - 2 \cdot 10^4 \text{ s}$	not given	2002	Ohkawachi



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Why to improve FY & Decay data for inventory and DH calculations ?



- Fast reactors: FY distribution depends on neutron spectrum

=> needs of FY measured at different neutron energies, as done per the GANIL team

=> Extra heat at short cooling time ?

=> needs of DH fission pulse measurements for $^{239}\text{Pu}_{\text{fast}}$ with lower uncertainties

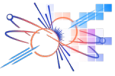
but also for other Pu isotopes



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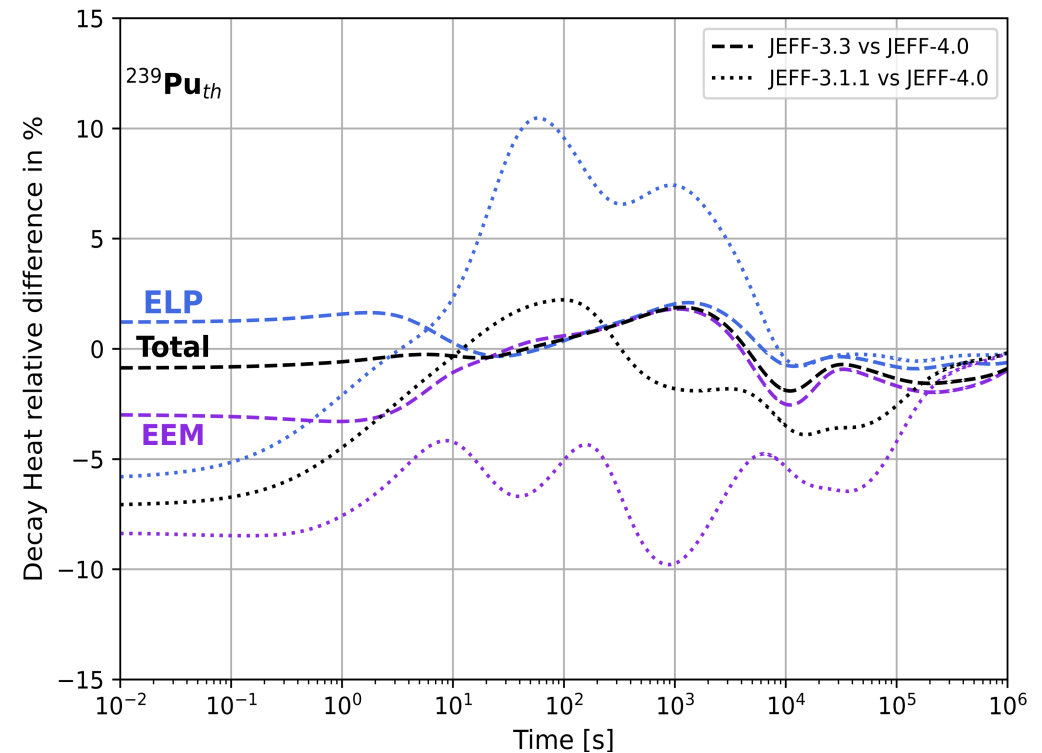
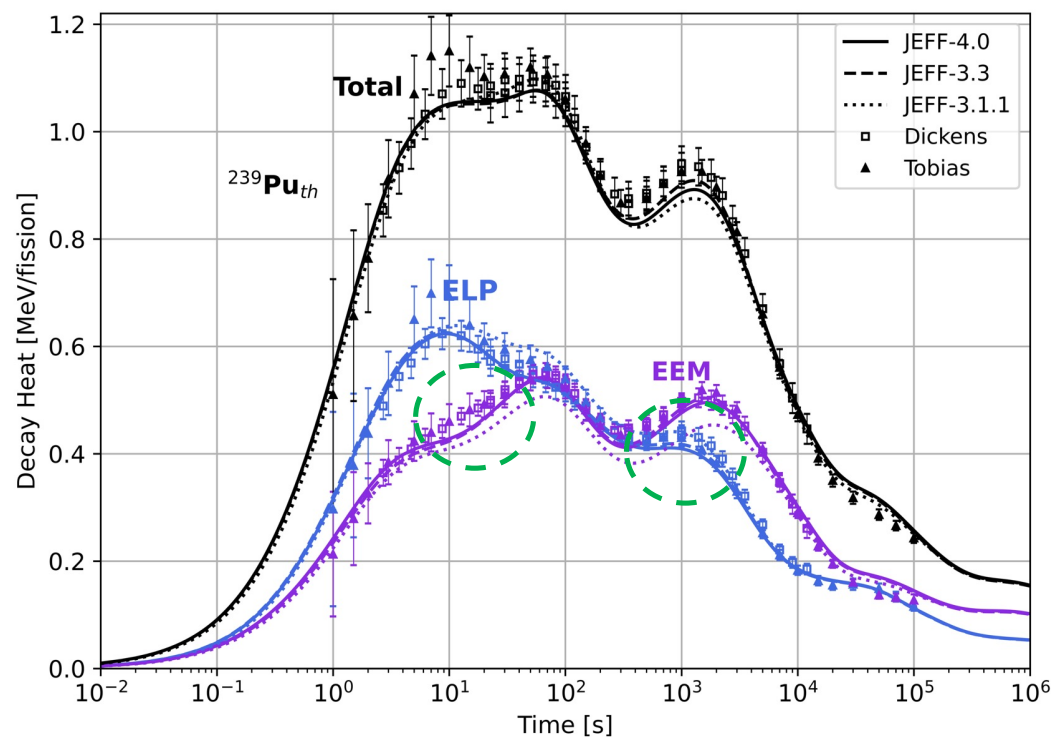
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Impact of new TAGS data in JEFF-4.0 decay data library : $^{239}\text{Pu}_{th}$



JEFF-3.3 new mean decay energies : ^{105}Mo , $^{104,105,106,107}\text{Tc}$, $^{87,88}\text{Br}$, $^{92,94}\text{Rb}$

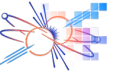
JEFF-4.0 new mean decay energies included : ^{93}Rb , $^{96gs,96m,99}\text{Y}$, $^{103,108}\text{Tc}$, ^{99}Y , ^{138}I , ^{142}Cs



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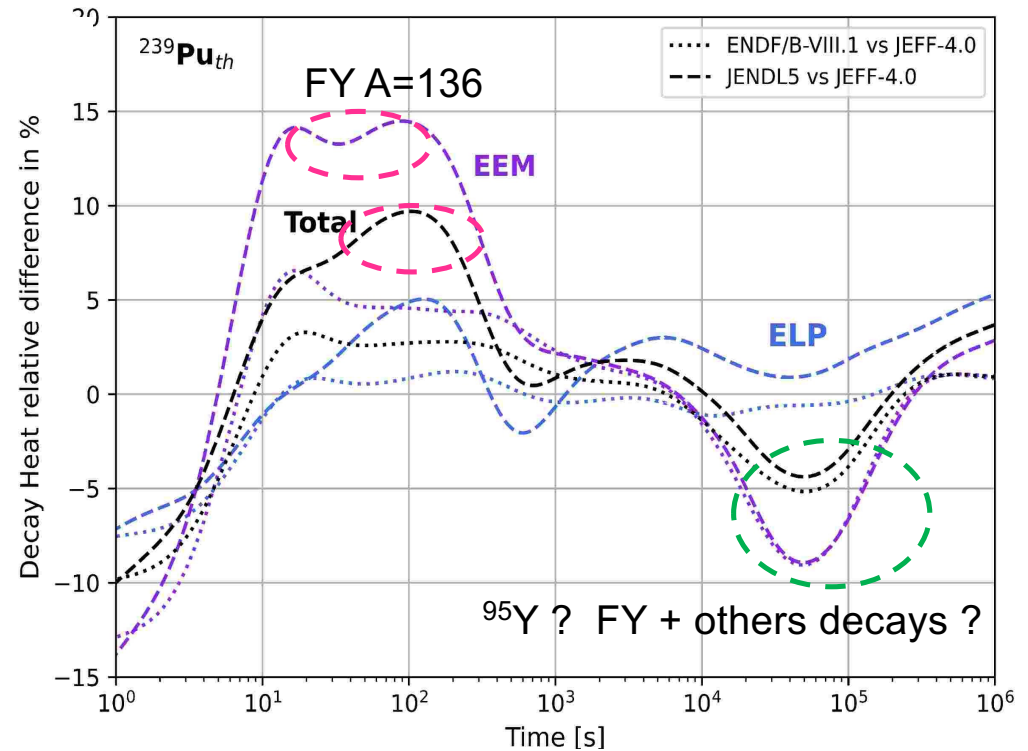
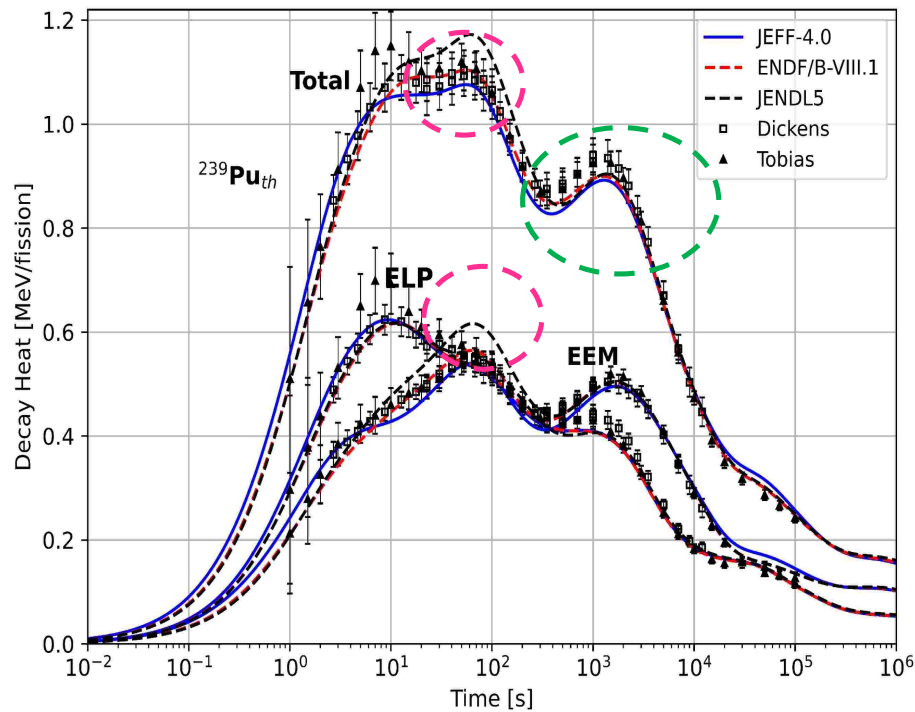
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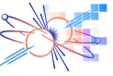
ENDF/B-VIII.1 (same than ENDF/B-VIII.0) new decays included : $^{82,83}\text{Ge}$, $^{82,86}\text{As}$, $^{88,89,90,91}\text{Br}$, ^{90}Kr , $^{93,95,96}\text{Rb}$, ^{95}Sr , $^{95,98,99}\text{Y}$, ^{134}Sb , ^{138}I , $^{140,141}\text{Cs}$, ^{142}Ba , $^{143,144,145}\text{La}$ *TAS published not in JEFF* *TAS published in JEFF*



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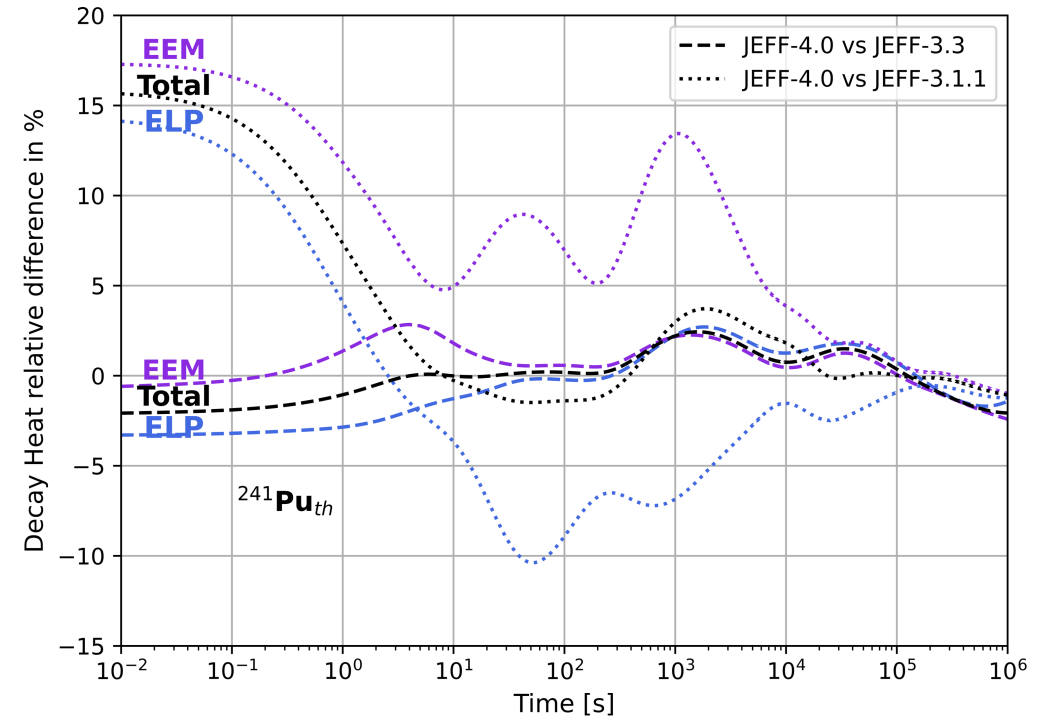
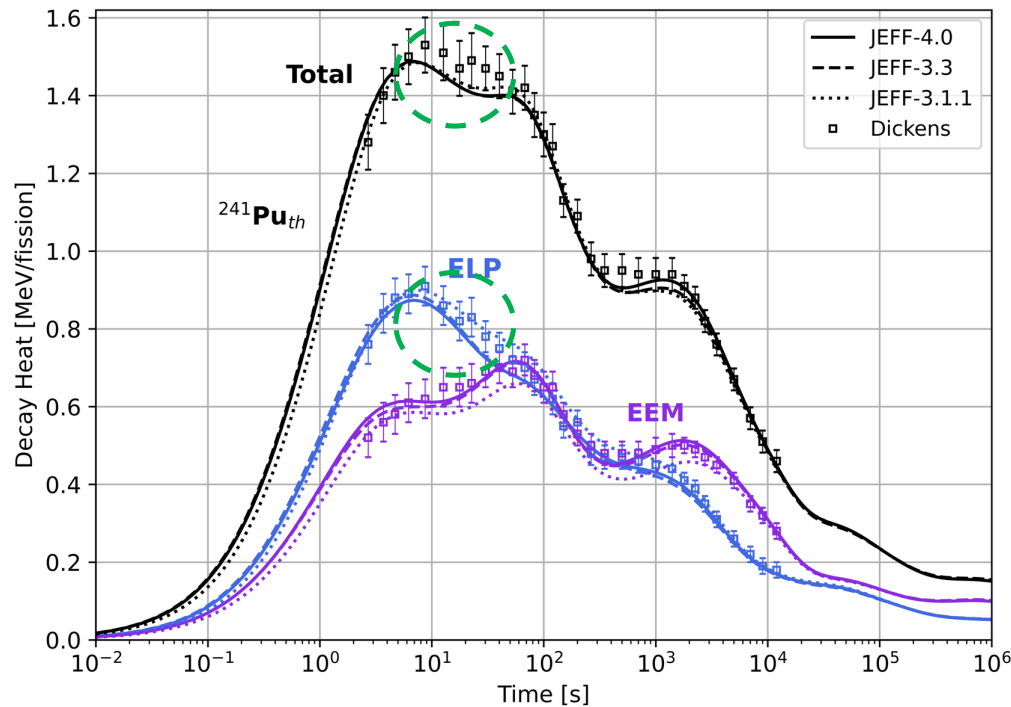
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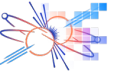
JEFF-4.0 new mean decay energies included : ^{93}Rb , $^{96\text{gs,m}},^{99}\text{Y}$, $^{103,108}\text{Tc}$, ^{99}Y , ^{138}I , ^{142}Cs



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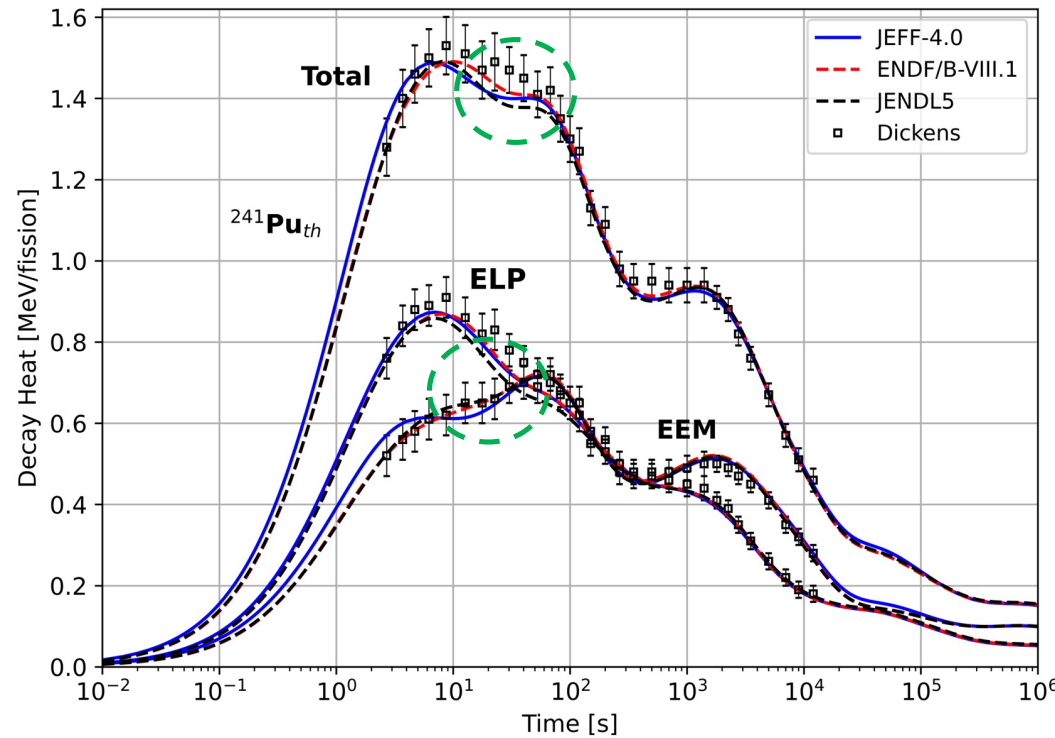
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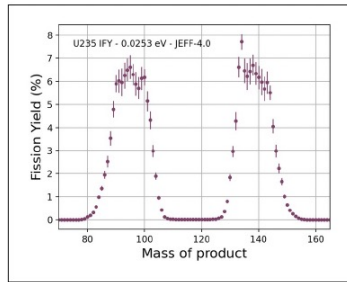
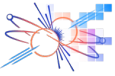
$^{93,95,96}\text{Rb}$, ^{95}Sr , $^{95,98,99}\text{Y}$, ^{134}Sb , ^{138}I , $^{140,141}\text{Cs}$, ^{142}Ba , $^{143,144,145}\text{La}$ *TAS published not in JEFF* *TAS published in JEFF*



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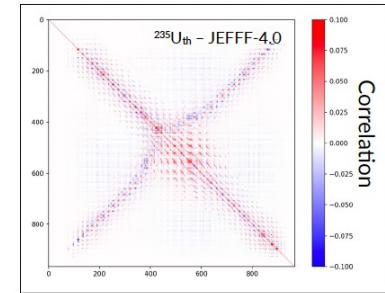
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ND uncertainty propagation – Monte Carlo approach



Input parameters and associated uncertainties
 $X = (x_1, x_2, x_3, \dots, x_n)^T$
 $\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, \dots, \sigma_{x_n}$

Covariance information (if present)
 $\sigma_{x_1 x_2}, \sigma_{x_1 x_3}, \dots, \sigma_{x_1 x_n}$
 $\sigma_{x_2 x_3}, \sigma_{x_2 x_4}, \dots, \sigma_{x_2 x_n}$
 $\dots$



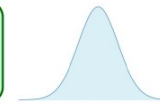
Sampling process

N perturbed input vectors of the type:
 $X^* = (x_1^*, x_2^*, x_3^*, \dots, x_n^*)^T$



Neutronic code: N calculations

N perturbed output vectors of the type:
 $Y^* = (y_1^*, y_2^*, y_3^*, \dots, y_m^*)^T$



Mean value and variance estimators

$\bar{y}_1, \bar{y}_2, \dots, \bar{y}_m$

$\sigma_{y_1}^2, \sigma_{y_2}^2, \dots, \sigma_{y_m}^2$

Code-to-code comparisons

Influence of the sampling distribution

Results with JEFF-4.0

Results using CEA's random fission yields

Recent work focussed on FY
See F. Esposito et al.,
WONDER 2026 proceeding

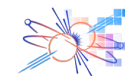
More complex cases



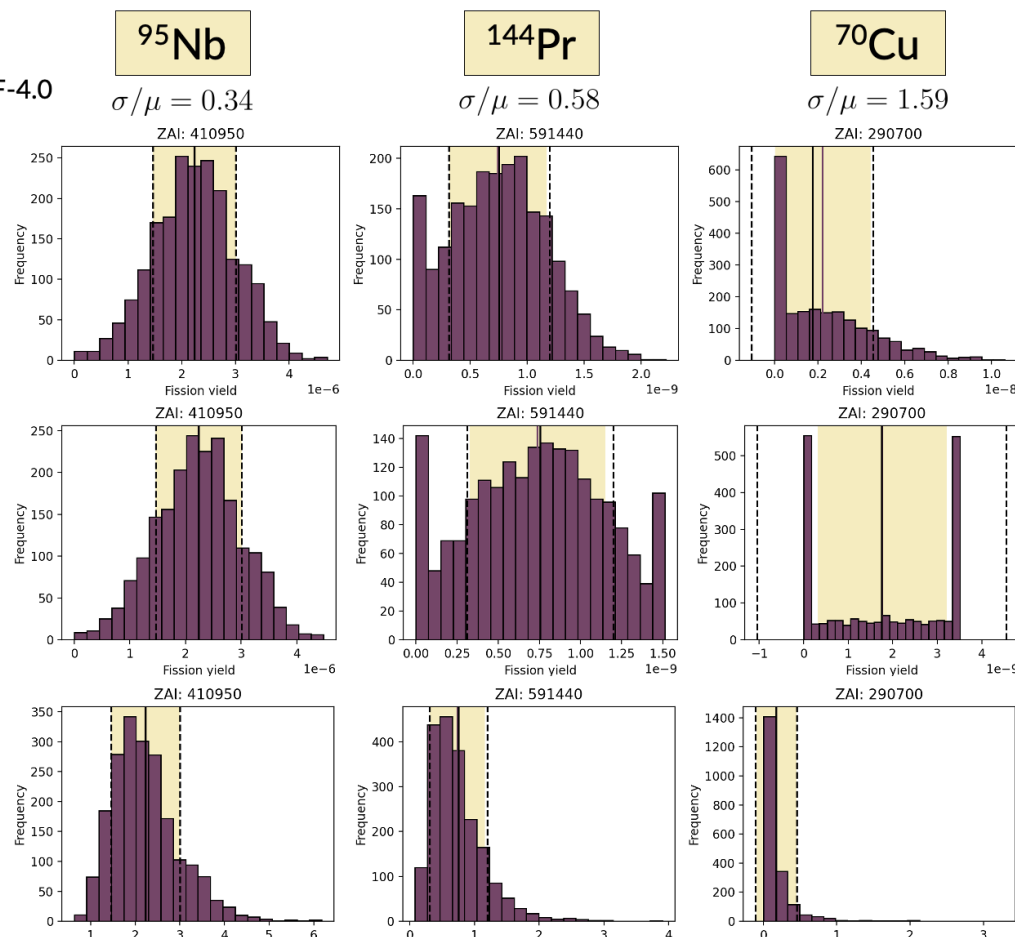
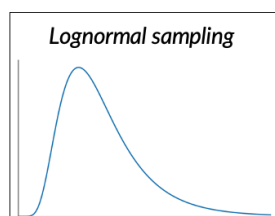
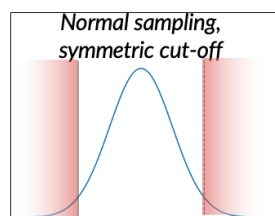
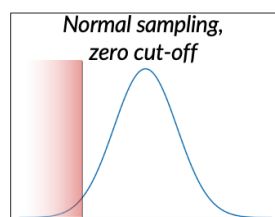
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FY uncertainty propagation : Influence of the sampling distribution



Different choices are possible on the sampling distribution and on the treatment of negative values. Example with 2000 samples, $^{235}\text{U}_{\text{th}}$, JEFF-4.0



Purple bins
Samples distribution

Purple solid line
Mean of the
samples

Yellow background
1 standard deviation
of the samples

Black solid line
Reference mean

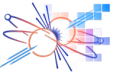
Black dashed line
Reference standard
deviation



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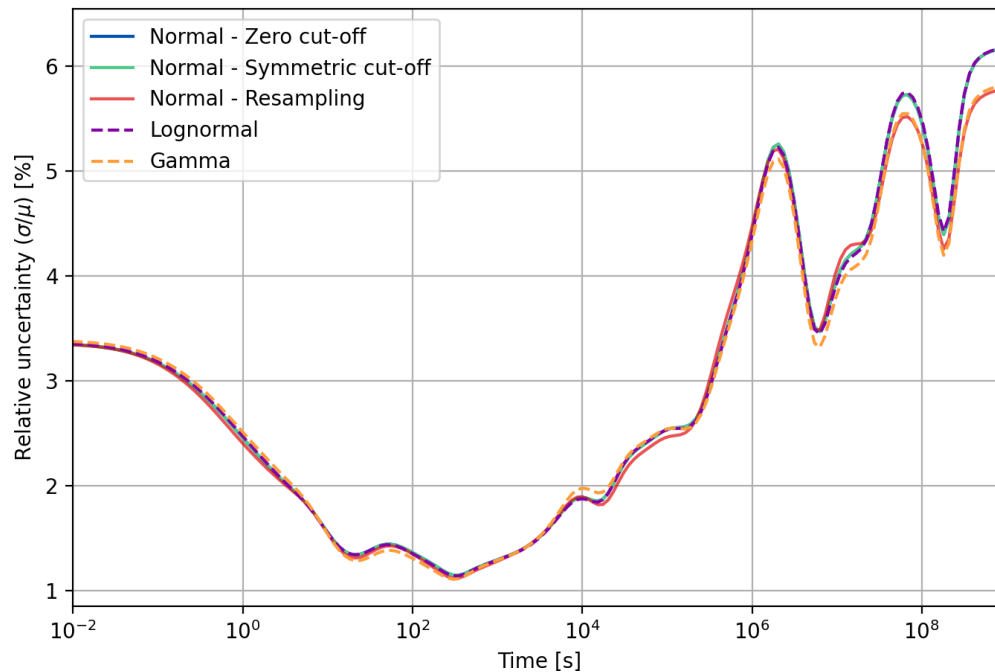
FY uncertainty propagation : Influence of the sampling distribution



Does the choice have an impact on the final decay heat uncertainty?

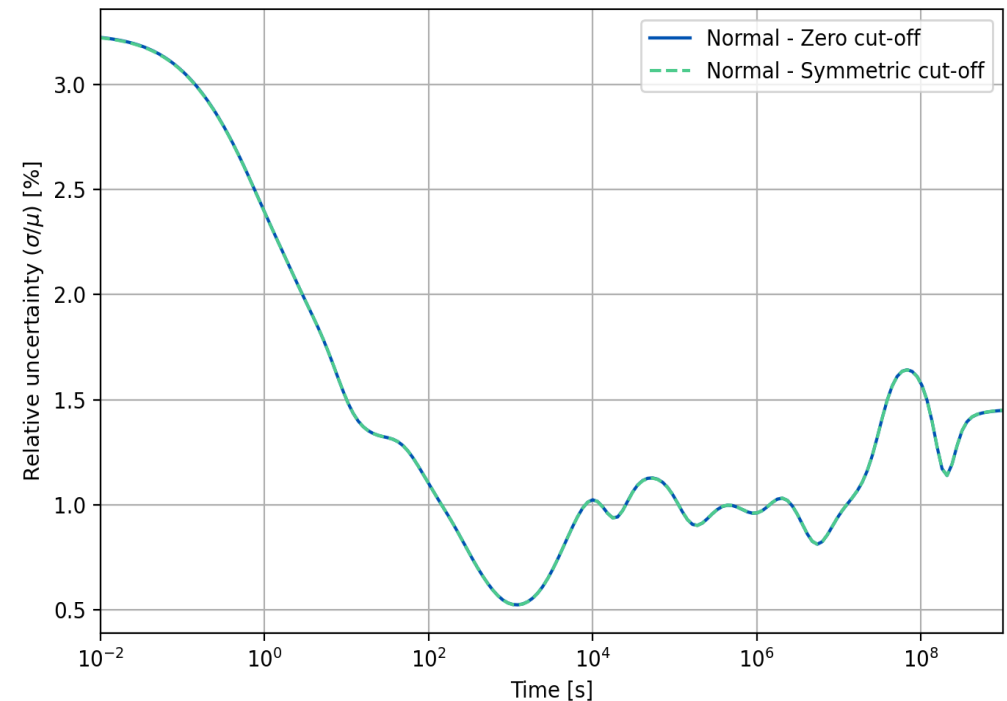
Test case: $^{239}\text{Pu}_{\text{th}}$ – JEFF-4.0 fission yields – 2000 samples

Without covariance matrix for fission yields



Max difference: <0.41%

With covariance matrix for fission yields



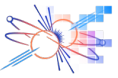
Max difference: <0.002%



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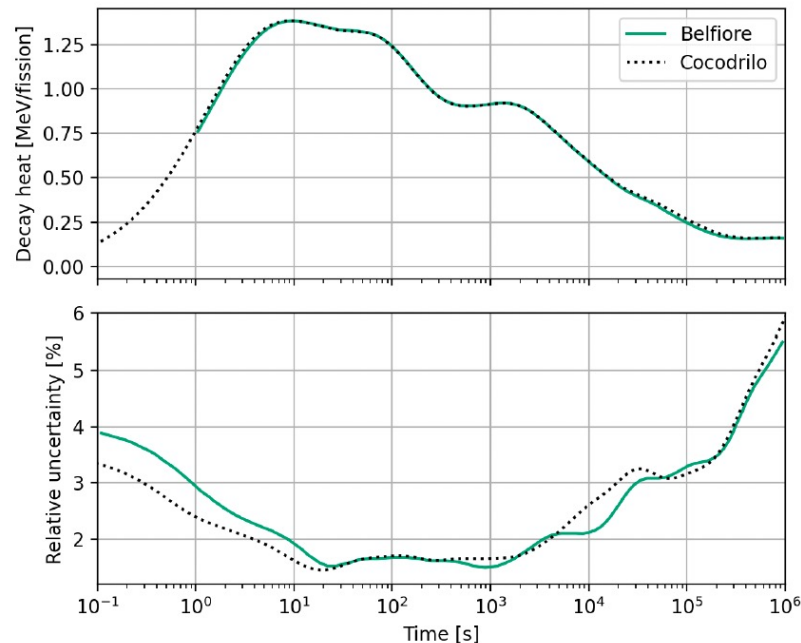
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FY uncertainty propagation : Code-to-code comparisons



Belfiore¹: Monte Carlo approach (SANDY code)

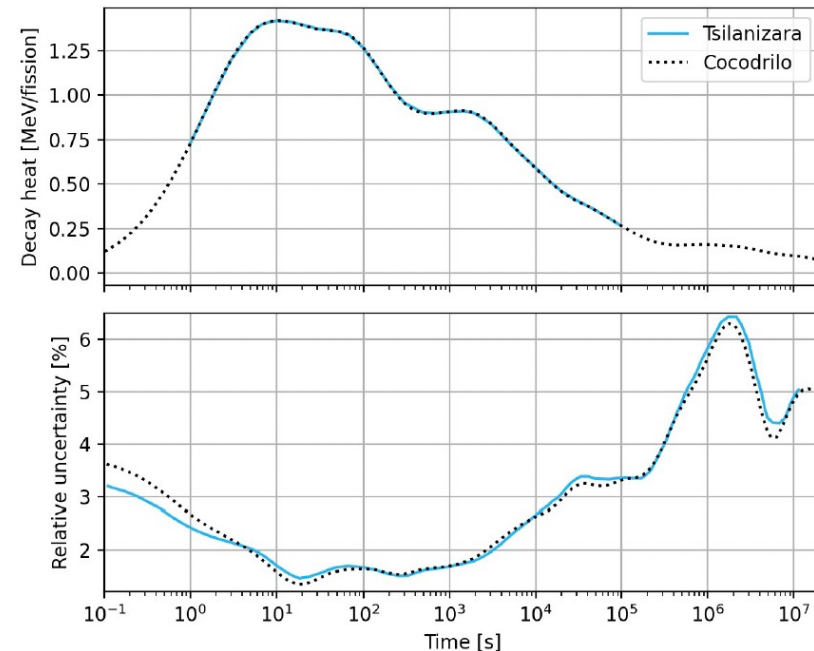
Fission Pulse from $^{235}\text{U}_{\text{th}}$ – JEFF-3.3. 200 samples with Normal sampling, symmetric cut-off. Differences may be explained by the small number of samples.



¹E. Belfiore. "Sensitivity and Uncertainty Analysis for Nuclear Data of Relevance in Spent Nuclear Fuel Characterization", Master Thesis, (2023)

Tsilanizara²: S/U approach

Fission Pulse from $^{235}\text{U}_{\text{th}}$ – JEFF-3.1.1. Differences may be explained by the different approach for uncertainties propagation.



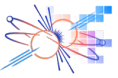
²A. Tsilanizara and T. Huynh. "New feature of DARWIN/PEPIN2 inventory code: Propagation of nuclear data uncertainties to decay heat and nuclide density". In: Annals of Nuclear Energy 164 (2021)



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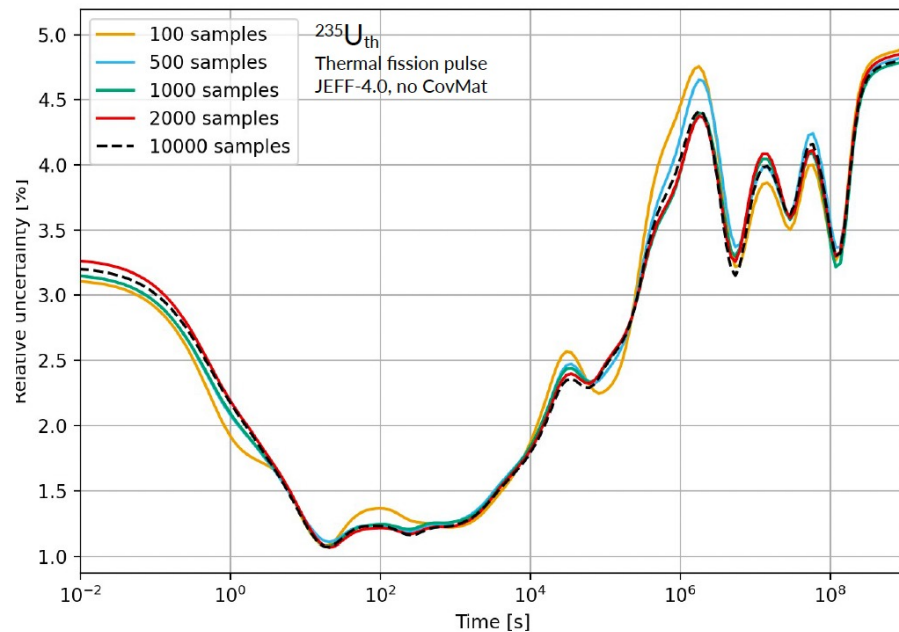
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FY uncertainty propagation : Code-to-code comparisons



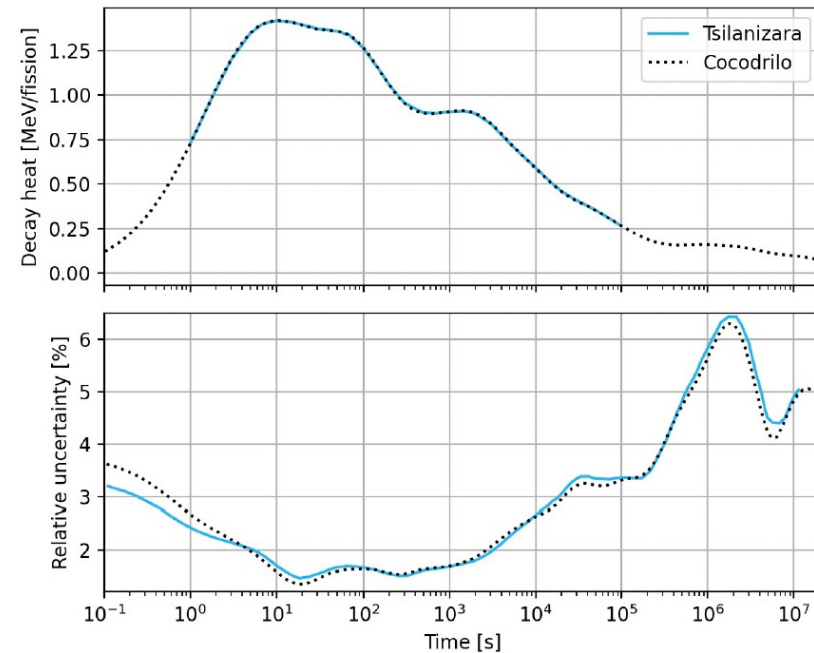
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Tsilanizara²: S/U approach

Fission Pulse from $^{235}\text{U}_{\text{th}}$ – JEFF-3.1.1. Differences may be explained by the different approach for uncertainties propagation.



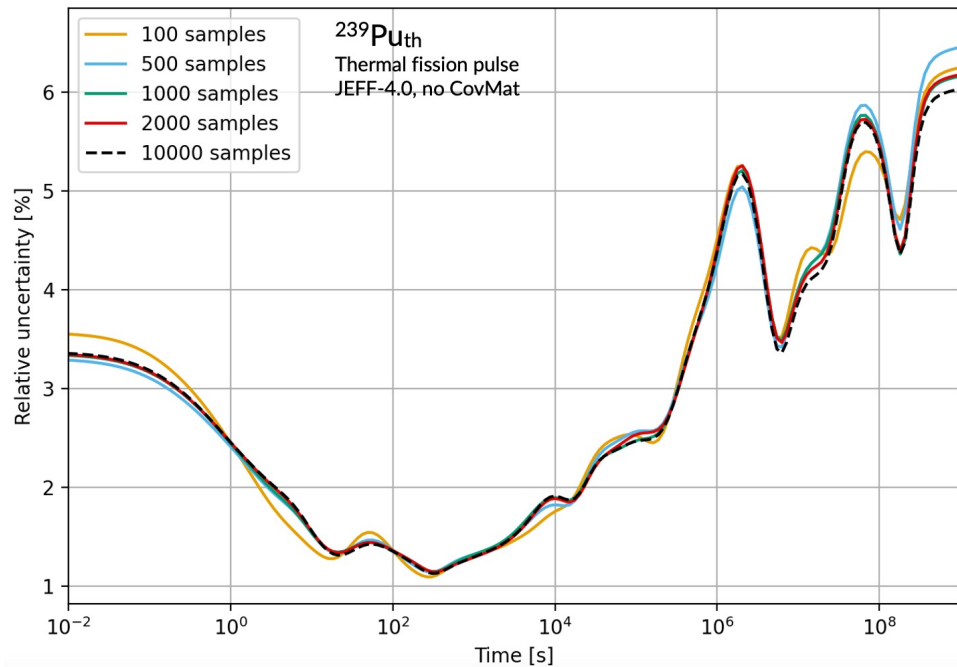
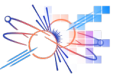
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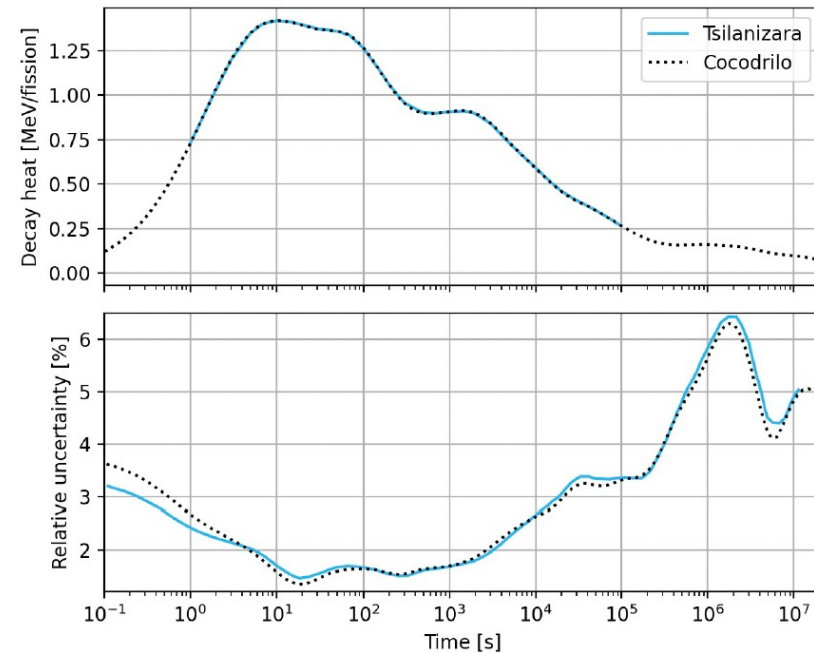
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FY uncertainty propagation : Code-to-code comparisons



Tsilanizara²: S/U approach

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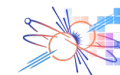
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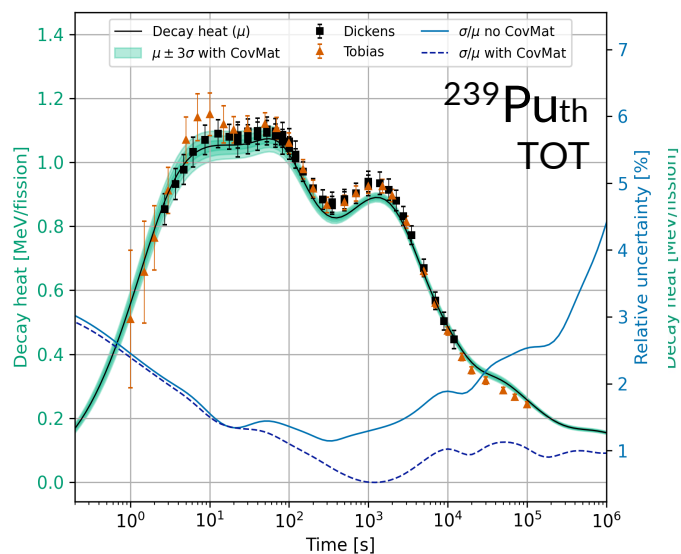
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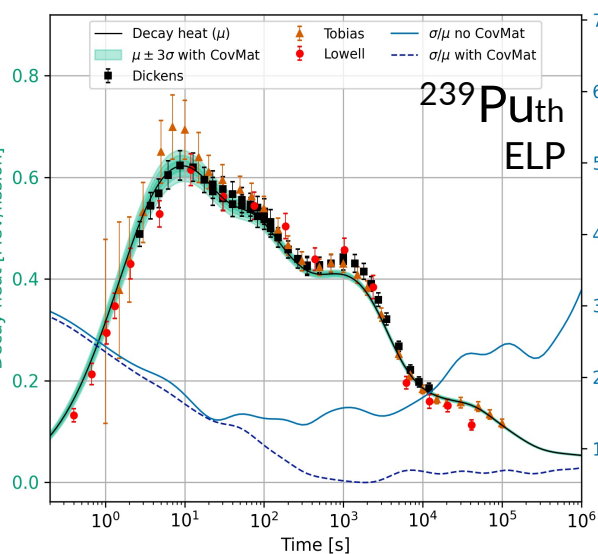
$^{239}\text{Pu}_{\text{th}}$ fission pulse decay heat – JEFF-4.0



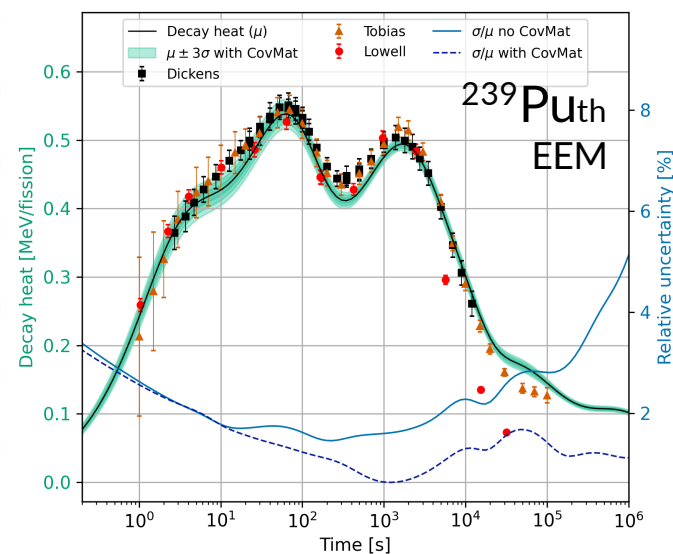
Total decay heat



Light particles component



Electromagnetic component



from Cocodrilo code, FY uncertainty only, 2000 samples,

Sampling method: Normal distribution, symmetric cut-off, w/o covariances matrices



μ = mean value

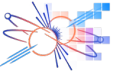
σ = standard deviation



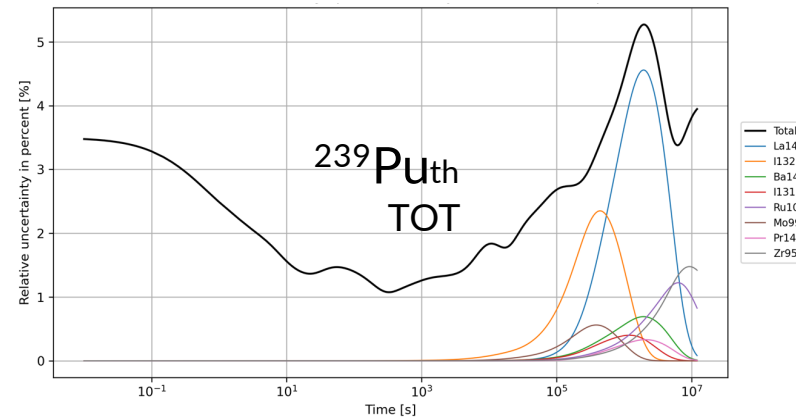
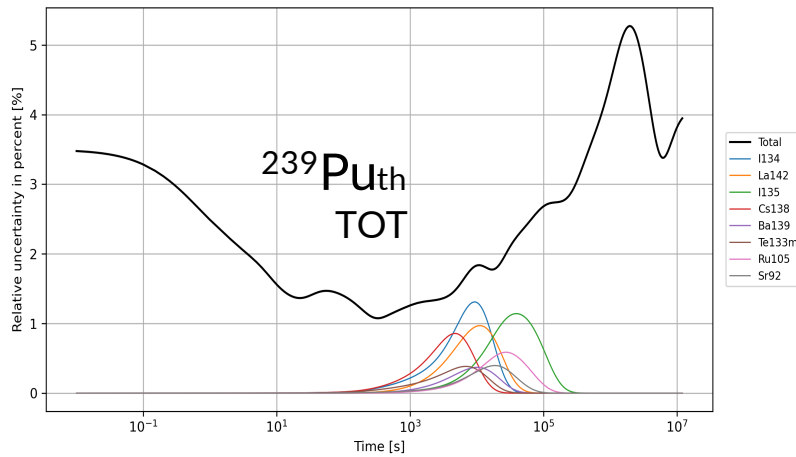
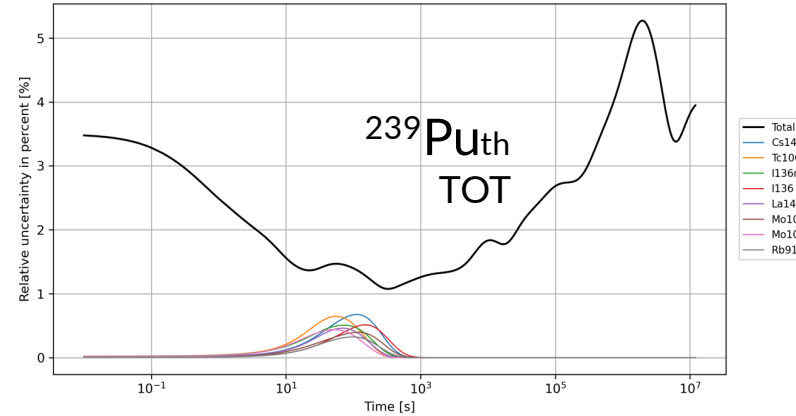
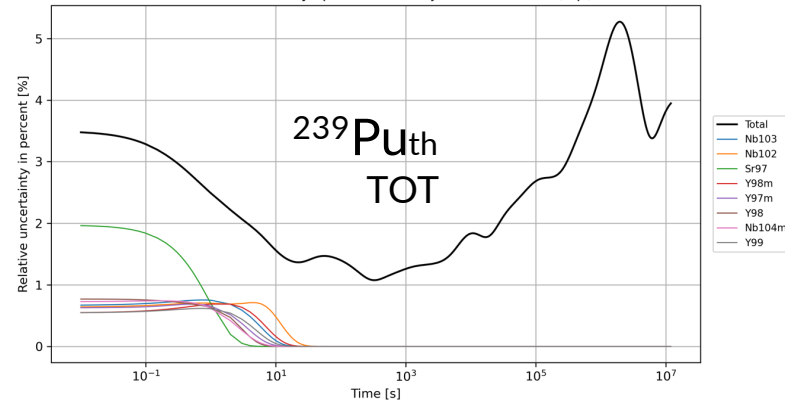
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$^{239}\text{Pu}_{\text{th}}$ fission pulse decay heat – Contribution of nuclides to uncertainty



JEFF-4.0+ FY sampling, no CovMat



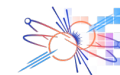
$^{99,103,105}\text{Mo}$
 ^{91}Rb
 $^{102,103,104\text{m}}\text{Nb}$
 $^{131,136,136\text{m}}\text{I}$
 ^{106}Tc
 $^{138,140}\text{Cs}$
 $^{140,144}\text{La}$
 ^{95}Zr
 $^{139,143}\text{Ba}$
 ^{103}Ru
 $^{140,144}\text{La}$
 $^{97\text{m},98,98\text{m},99}\text{Y}$
 $^{97,92}\text{Sr}$



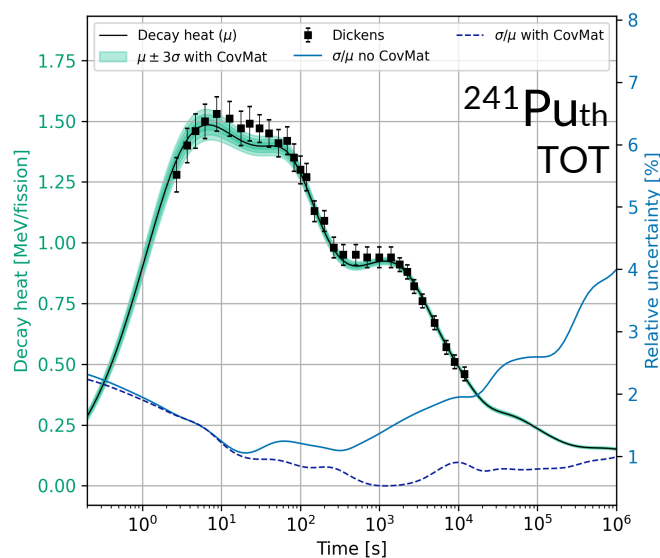
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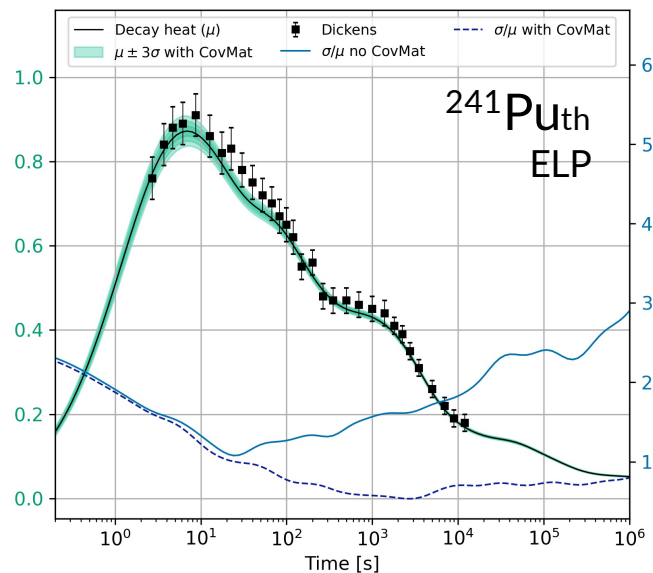
$^{241}\text{Pu}_{\text{th}}$ fission pulse decay heat – JEFF-4.0



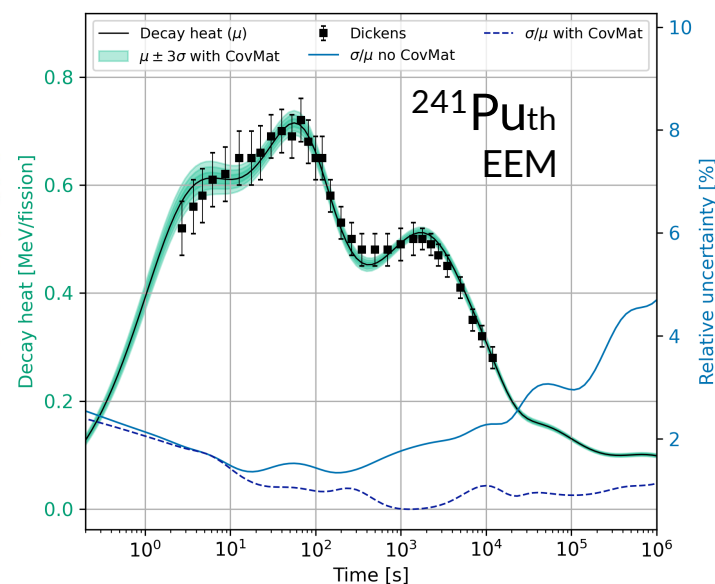
Total decay heat



Light particles component



Electromagnetic component



from Cocodrilo code, FY uncertainty only, 2000 samples,

Sampling method: Normal distribution, symmetric cut-off, w/o covariances matrices



μ = mean value

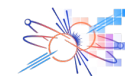
σ = standard deviation



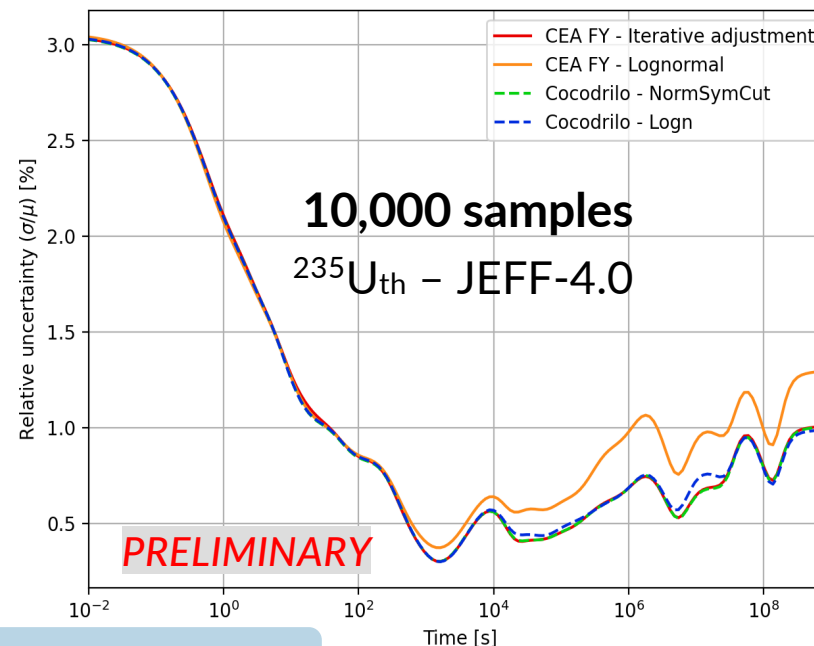
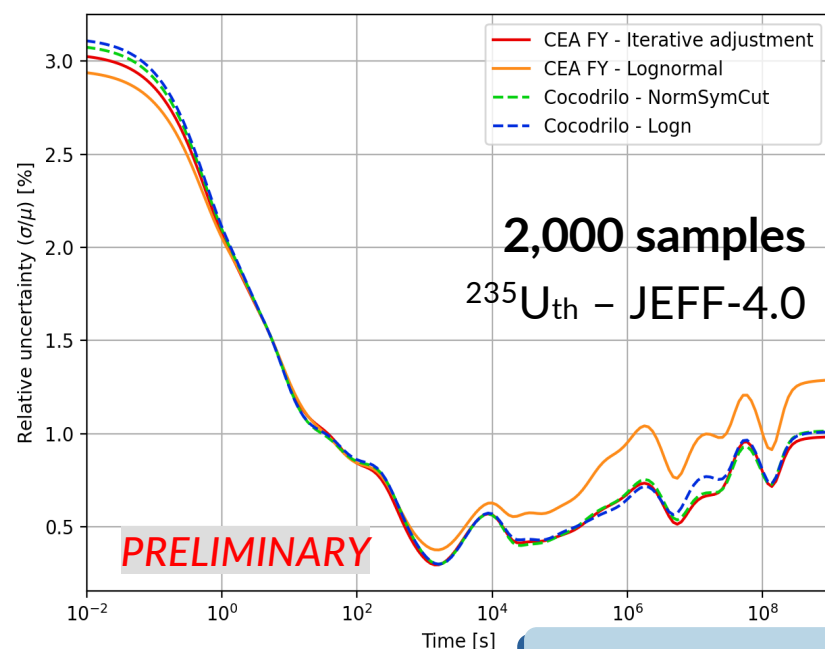
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FY uncertainty propagation – using CEA's already sampled FY files



Results directly using samples generated by CEA¹: JEFF-4.0 files made available in April 2026 within APRENDE for Independent Fission Yields on 4 thermal systems. They are **10'000 samples with constrain on Cumulative Fission Yields**.



Max difference: ~0.35% for both cases

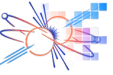
¹G. Kessedjian et al., "Monte Carlo Fission Yield files for the 4 major fissile nuclei", Nuclear Data Week - JEFF meeting / APRENDE, 13-17 April 2026



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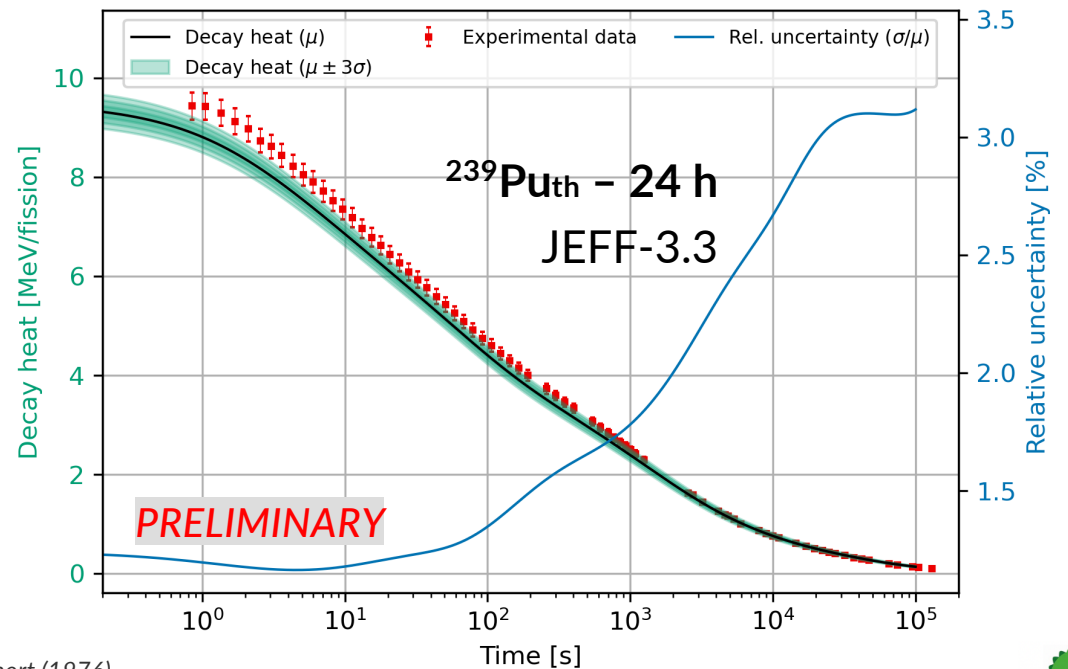
More complex cases foreseen: Irradiation of samples with water moderated ^{252}Cf source



Collaborative work with Sofia Portolan (PSI, EPFL), Dimitri Rochman (NAGRA)

- Experimental program supported per EPRI (Friesenhahn et al. 1976,1979)
- Decay heat measurements available for longer irradiation times than fission pulses

Target	Irradiation time	Cooling time
^{235}U	24 hours	1s - 1.8 days
^{235}U	35 days	1s - 2.4 days
^{235}U	1 000 s	1s - 0.6 days
^{235}U	20 000 s	1s - 1.2 days
^{239}Pu	24h	1s - 1.5 days
^{239}Pu	1 000s	1s - 5500 s



¹S. J Friesenhahn et al., ^{235}U Fission Product Decay Heat from 1 to 105 seconds, EPRI report (1976).

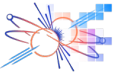
²S. J Friesenhahn et al., Measurement of ^{239}Pu and ^{235}U Fission Product Decay Power From 1 to 105 Seconds, EPRI report (1979).



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Conclusions and Outlooks



- Impact of new TAGS data on DH calculations => needs of new DH fission pulses measurements for Pu isotopes
 - Development of **Cocodrilo code** with studies on FY samplings
 - First application to the new **JEFF-4.0** library release and covariance matrices
 - Very **small impact** of the chosen sampling distribution on fission pulse calculations
 - Tools ready for more detailed studies
-
- Take over previous studies on Decay Data sampling with Cocodrilo
 - Automatized tools to identify Pandemonium nuclei (J. Halwani Phd on MSR) applied now to thermal fission pulses
 - More complex cases (pincell, PWR assemblies, MSR case) => coupling with Coconust (A. Laureau, LPSC)

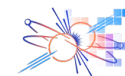


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**Thank you for
your attention**

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GANIL: Fanny Farget, Diego Ramos

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NAGRA: Dimitri Rochman **PSI:** Sofia Portolan

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TAS collaboration : IFIC Valencia, SEN team@Subatech, Univ. of Surrey)

For collaborative work or scientific discussions !



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Get in touch for more information:



<https://aprende-project.eu/>



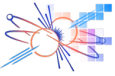
contact@aprende-project.eu

Thank you!



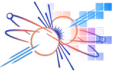
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Procedure used per CEA for FY sampling

SetZero

$$G(\mathbf{Y}; \bar{\mathbf{y}}; \Sigma) \text{ and } \sigma_i^2 = \Sigma_{ii}$$

- spectral decomposition

$$\Sigma = \mathbf{P} \cdot \mathbf{D} \cdot \mathbf{P}^T$$

- Sampling

$$\mathbf{S} \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$$

$$\mathbf{y}_s = \bar{\mathbf{y}} + \mathbf{P} \cdot \mathbf{D}^{1/2} \cdot \mathbf{S}$$

- Regularization

$$\text{if } y_{s,i} < 0; y_{s,i} = 0$$

LogNormal

$$\bar{y}_i^{LN} = \log \left(\frac{\bar{y}_i^2}{\sigma_i^2 + \bar{y}_i^2} \right) \quad (\sigma_i^{LN})^2 = \log \left(1 + \frac{\sigma_i^2}{\bar{y}_i^2} \right)$$

$$\Sigma_{ij}^{LN} = \log \left(1 + \frac{\Sigma_{ij}}{\bar{y}_i \cdot \bar{y}_j} \right)$$

- Regularization

$$\text{Arg} > 0$$

$$\text{Arg} < 0$$

$$\Sigma_{ij}^{log} \approx \frac{\Sigma_{ij}}{\sigma_i \cdot \sigma_j} \cdot \sigma_i^{LN} \cdot \sigma_j^{LN}$$

Corr_{ij}

- Sampling

$$\Sigma^{LN} = \mathbf{P} \cdot \mathbf{D} \cdot \mathbf{P}^T$$

$$\mathbf{y}_s^{LN} = \bar{\mathbf{y}}^{LN} + \mathbf{P} \cdot \mathbf{D}^{1/2} \cdot \mathbf{S}$$

$$\mathbf{S} \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$$

$$y_{s,i} = \exp(y_{s,i}^{LN})$$

iterative adjustment

- Cholesky decomposition

$$\text{Find } \mathbf{L} : \text{Cov}_{\mathbf{Y}} = \mathbf{L} \mathbf{L}^T$$

- Sampling

$$\mathbf{S} \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$$

$$\mathbf{y}_s = \bar{\mathbf{y}} + \mathbf{L} \cdot \mathbf{S}$$

- Regularization

$$\mathbf{y}_s = |\mathbf{y}_s|$$

- k Iterative process

$$y_{s,i}^k = \left| \left(y_{s,i}^{k-1} - \bar{y}_{s,i}^{k-1} \right) \cdot \frac{\sigma_i}{\sigma_{y_{s,i}^{k-1}}} + \bar{y}_i \right|$$



G. Kessedjian et al. - Nuclear Data Week - JEFF meeting / APRENDE, 13-17 April 2026

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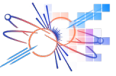
Slide taken from: S. M. Cheikh, A. Chebboubi, G. Kessedjian, O. Serot, D. Bernard, *Monte Carlo Fission Yield files for the 4 major fissile nuclei*, Nuclear Data Week - JEFF meeting / APRENDE, 13-17 April 2026



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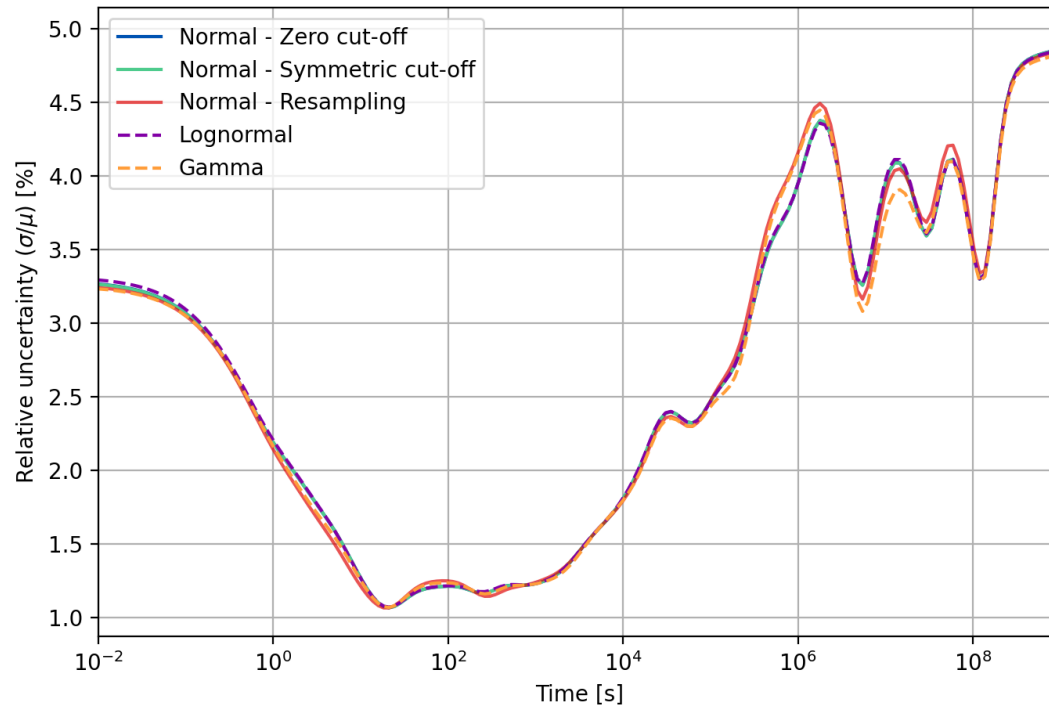
FY uncertainty propagation : Influence of the sampling distribution



Does the choice have an impact on the final decay heat uncertainty?

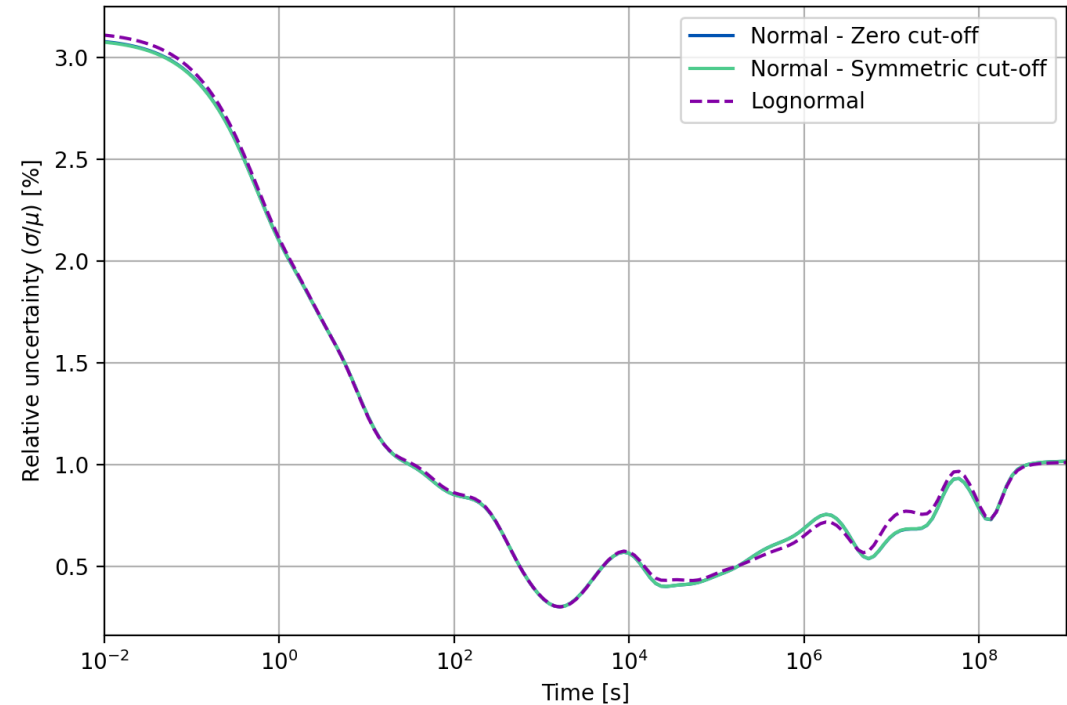
Test case: $^{235}\text{U}_{\text{th}}$ – JEFF-4.0 fission yields – 2000 samples

Without covariance matrix for fission yields



Max difference: <0.3%

With covariance matrix for fission yields



Max difference: <0.15%



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