WONDER 2026

Impact of nuclear data on decay heat calculations

Francesco Esposito

esposito@subatech.in2p3.fr

PhD director: **Lydie Giot**

02 / 07 / 2026

International Workshop On Nuclear Data Evaluation for Reactor Applications

Aix-en-Provence, France

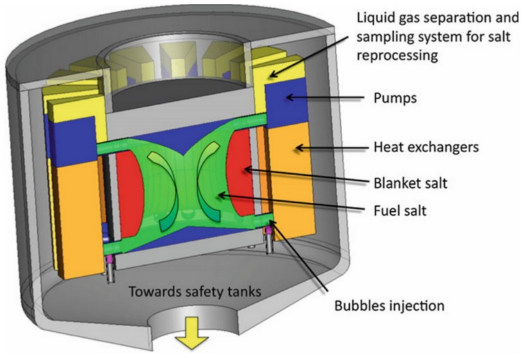
June 29th – July 3rd, 2026

Decay heat and uncertainties

Decay heat importance

Decay heat can be defined as the *recoverable energy released from the decay of radionuclides after the reactor shutdown*. It constitutes an **important source of power** over a wide time scale.

Decay heat is a fundamental safety function for the fuel cycle back-end.



E. Merle-Lucotte et al. (2016)

Innovative reactor concepts

GenIV → MSR

↓

Unique operational conditions and geometries

↓

Need to expand research on decay heat calculation and uncertainty propagation

Classical methods for decay heat calculation cannot be used

Lack of return of experience

Different back-end fuel cycle with respect to solid fuel

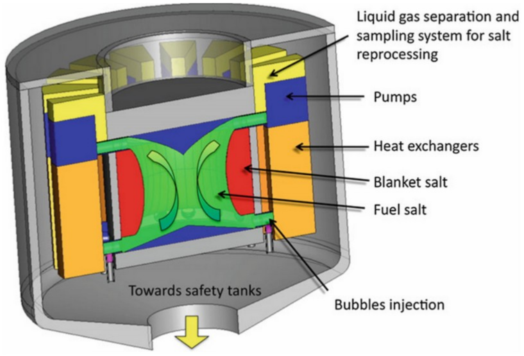
MSR = Molten Salt Reactor

Decay heat and uncertainties

Decay heat importance

Decay heat can be defined as the *recoverable energy released from the decay of radionuclides after the reactor shutdown*. It constitutes an **important source of power** over a wide time scale.

Decay heat is a fundamental safety function for the fuel cycle back-end.



E. Merle-Lucotte et al. (2016)

Innovative reactor concepts

GenIV → MSR

↓

Unique operational conditions and geometries

↓

Need to expand research on decay heat calculation and uncertainty propagation

Classical methods for decay heat calculation cannot be used

Lack of return of experience

Different back-end fuel cycle with respect to solid fuel

MSR = Molten Salt Reactor

Uncertainty propagation

Safety authorities require not only the decay heat value, but also the associated **uncertainty**.

$$\frac{dN_i(t)}{dt} = \sum_{j\neq i}^{M} \left[N_j(t) \left(b_{j\to i}\lambda_j + \sum_p \phi_p(t)\langle\sigma_{p,j\to i}\rangle \right) - N_i(t) \left(\lambda_i + \sum_p \phi_p(t)\langle\sigma_{p,i\to j}\rangle \right) \right]$$

Studies of Subatech (Nantes) and LPSC (Grenoble): develop **flexible** codes for MSR simulation with uncertainty propagation **from nuclear data.**

COCODRILO
Sampling FY, λ, E_{mean}
F. Esposito, Y. Molla

COCONUST
Sampling XS, ν, ...
A. Laureau[1]

→

CEREIS
MSR modeling
J. Halwani[2]

→

Safety parameters
Inventory
Decay heat

[1] *A. Laureau et al. Uncertainty propagation for the design study of the PETALE experimental programme in the CROCUS reactor (2020)*

[2] *J. Halwani, Decay Heat Calculations and Application of the Lines of Defence Method to Chloride Molten Salt Reactor ARAMIS-A (2025)*

Monte Carlo method for uncertainty propagation

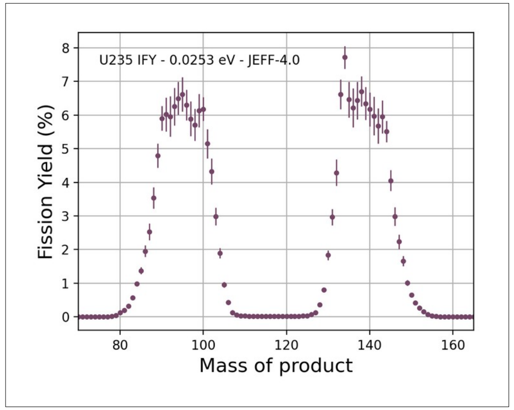
Input parameters and associated uncertainties

$$X = (x_1, x_2, x_3, ..., x_n)^T$$
$$\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, ..., \sigma_{x_n}$$

Covariance information (if present)

$\sigma_{x_1x_2}, \sigma_{x_1x_2}, \sigma_{x_1x_2}, ..., \sigma_{x_1x_n}$
$\sigma_{x_2x_3}, \sigma_{x_2x_4}, ..., \sigma_{x_2x_n}$
$\cdots$

Monte Carlo method for uncertainty propagation

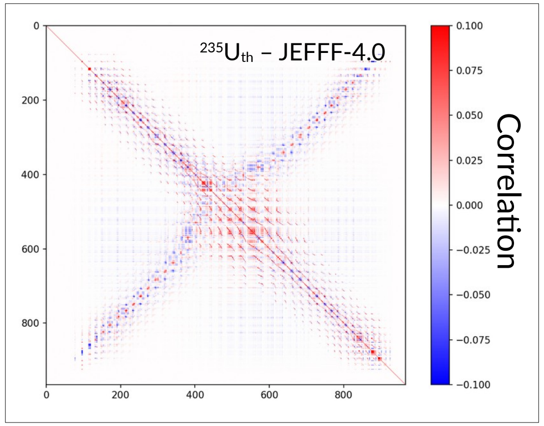


Input parameters and associated uncertainties

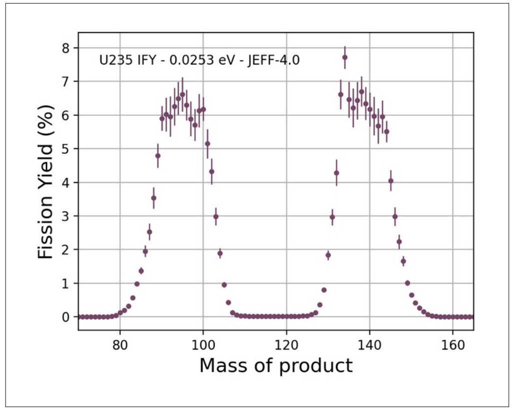
$$X = (x_1, x_2, x_3, ..., x_n)^T$$
$$\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, ..., \sigma_{x_n}$$

Covariance information (if present)

$\sigma_{x_1x_2}, \sigma_{x_1x_2}, \sigma_{x_1x_2}, ..., \sigma_{x_1x_n}$
$\sigma_{x_2x_3}, \sigma_{x_2x_4}, ..., \sigma_{x_2x_n}$
...



Monte Carlo method for uncertainty propagation

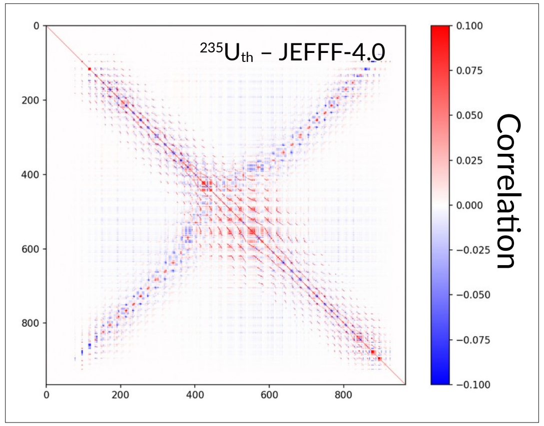


Input parameters and associated uncertainties

$$X = (x_1, x_2, x_3, ..., x_n)^T$$
$$\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, ..., \sigma_{x_n}$$

Covariance information (if present)

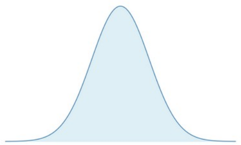
$$\sigma_{x_1x_2}, \sigma_{x_1x_2}, \sigma_{x_1x_2}, ..., \sigma_{x_1x_n}$$
$$\sigma_{x_2x_3}, \sigma_{x_2x_4}, ..., \sigma_{x_2x_n}$$
$$...$$



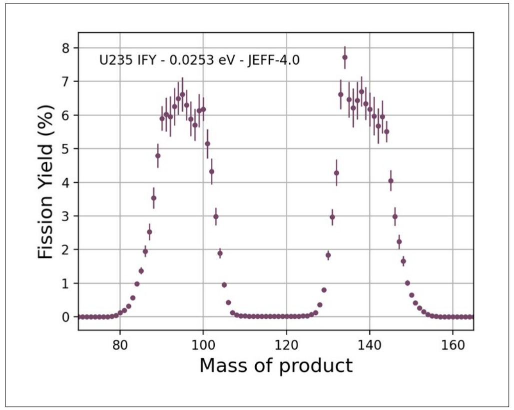
Sampling process

N perturbed input vectors of the type:

$$X^* = (x_1^*, x_2^*, x_3^*, ..., x_n^*)^T$$



Monte Carlo method for uncertainty propagation

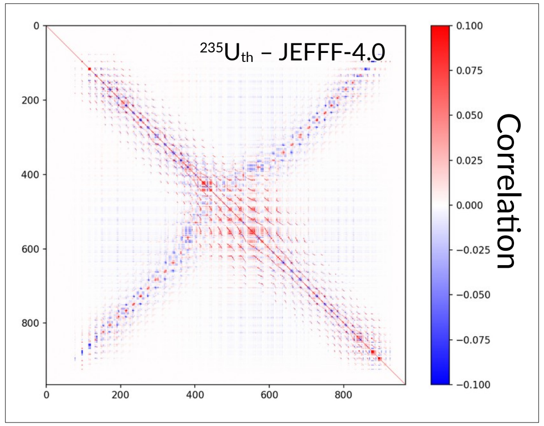


Input parameters and associated uncertainties

$$X = (x_1, x_2, x_3, \dots, x_n)^T$$
$$\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, \dots, \sigma_{x_n}$$

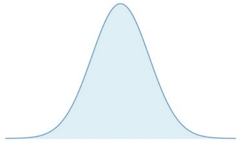
Covariance information (if present)

$$\sigma_{x_1x_2}, \sigma_{x_1x_2}, \sigma_{x_1x_2}, \dots, \sigma_{x_1x_n}$$
$$\sigma_{x_2x_3}, \sigma_{x_2x_4}, \dots, \sigma_{x_2x_n}$$
$$\dots$$



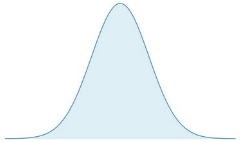
Sampling process

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

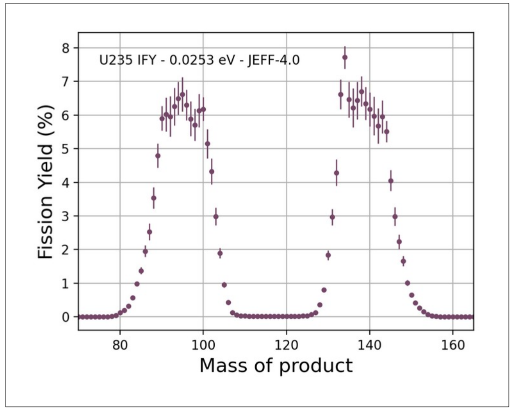


Neutronic code: N calculations

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



Monte Carlo method for uncertainty propagation

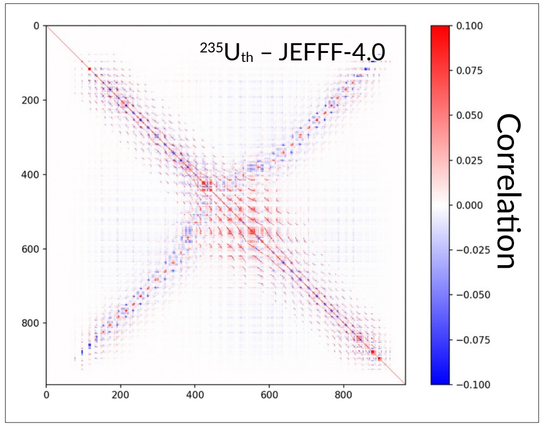


Input parameters and associated uncertainties

$$X = (x_1, x_2, x_3, \dots, x_n)^T$$
$$\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, \dots, \sigma_{x_n}$$

Covariance information (if present)

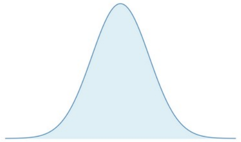
$$\sigma_{x_1x_2}, \sigma_{x_1x_2}, \sigma_{x_1x_2}, \dots, \sigma_{x_1x_n}$$
$$\sigma_{x_2x_3}, \sigma_{x_2x_4}, \dots, \sigma_{x_2x_n}$$
$$\dots$$



Sampling process

N perturbed input vectors of the type:

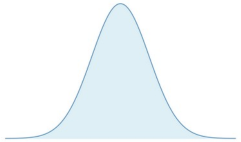
$$X^* = (x_1^*, x_2^*, x_3^*, \dots, x_n^*)^T$$



Neutronic code: N calculations

N perturbed output vectors of the type:

$$Y^* = (y_1^*, y_2^*, y_3^*, \dots, y_m^*)^T$$

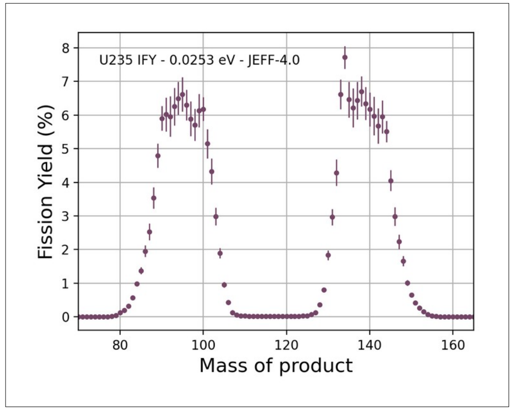


Mean value and variance estimators

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

$\sigma_{y1}^2, \sigma_{y2}^2, \dots, \sigma_{ym}^2$

Monte Carlo method for uncertainty propagation

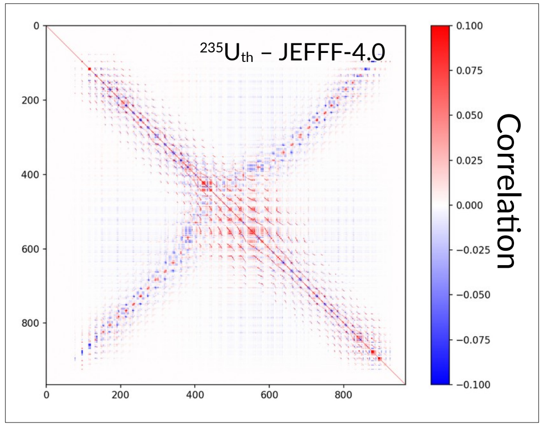


Input parameters and associated uncertainties

$$X = (x_1, x_2, x_3, \ldots, x_n)^T$$
$$\sigma_{x_1}, \sigma_{x_2}, \sigma_{x_3}, \ldots, \sigma_{x_n}$$

Covariance information (if present)

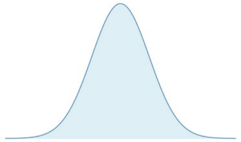
$$\sigma_{x_1x_2}, \sigma_{x_1x_2}, \sigma_{x_1x_2}, \ldots, \sigma_{x_1x_n}$$
$$\sigma_{x_2x_3}, \sigma_{x_2x_4}, \ldots, \sigma_{x_2x_n}$$
$$\ldots$$



Sampling process

N perturbed input vectors of the type:

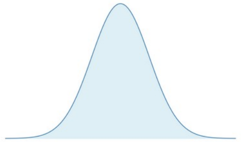
$$X^* = (x_1^*, x_2^*, x_3^*, \ldots, x_n^*)^T$$



Neutronic code: N calculations

N perturbed output vectors of the type:

$$Y^* = (y_1^*, y_2^*, y_3^*, \ldots, y_m^*)^T$$



Mean value and variance estimators

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

$$\sigma^2_{y_1}, \sigma^2_{y_2}, \ldots, \sigma^2_{y_m}$$

Code-to-code comparisons

Influence of the sampling distribution

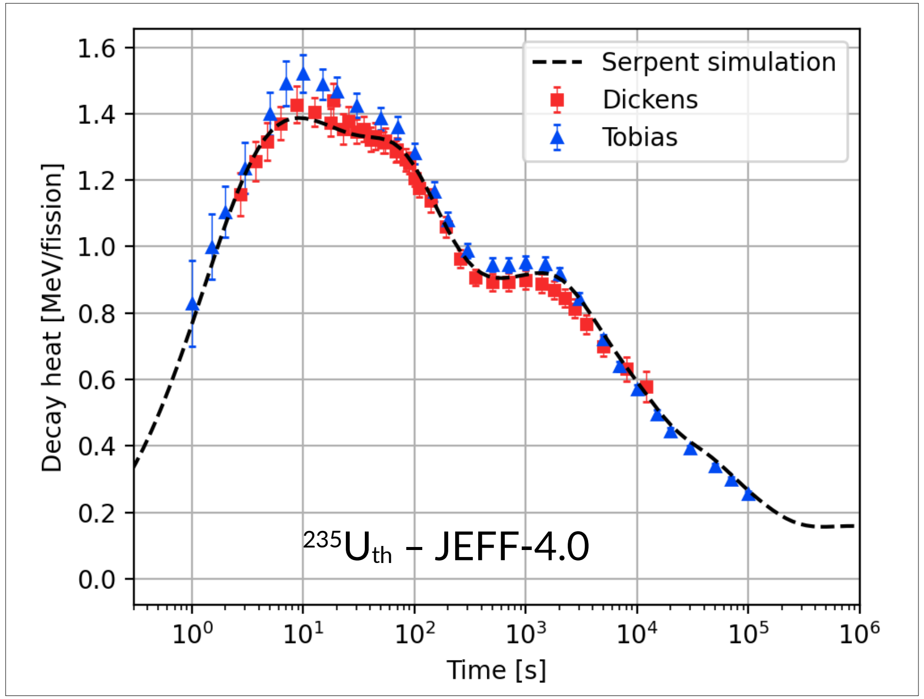
Results with JEFF-4.0

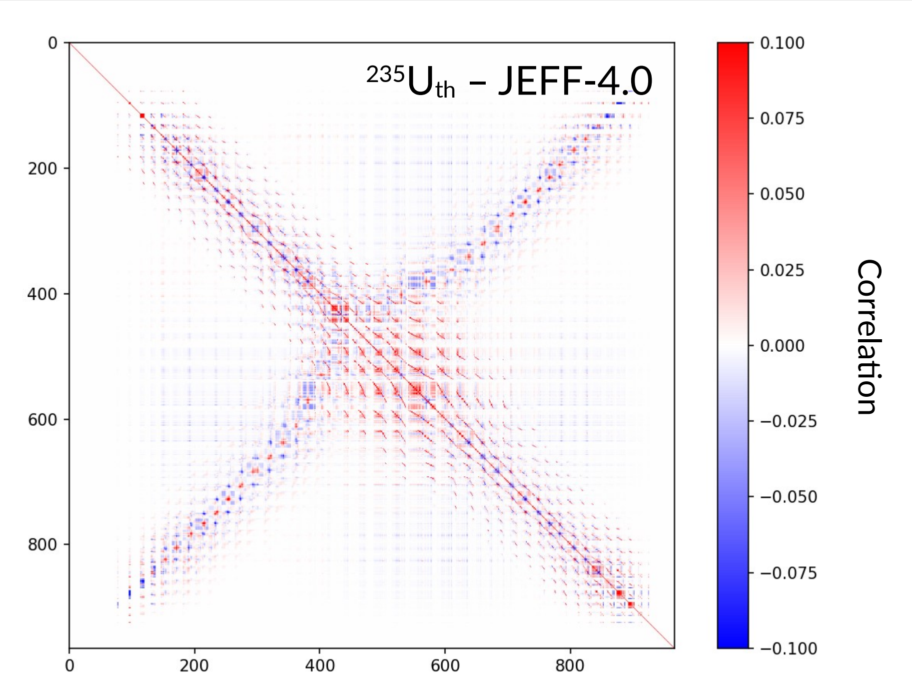
Results using CEA's random fission yields

Results with other libraries and impact of TAGS measurements

More complex cases

Fission pulse decay heat





Fission pulse decay heat

- Large availability of experimental data for thermal cases
- Disentangle fission yields and decay data contribution from that of cross sections

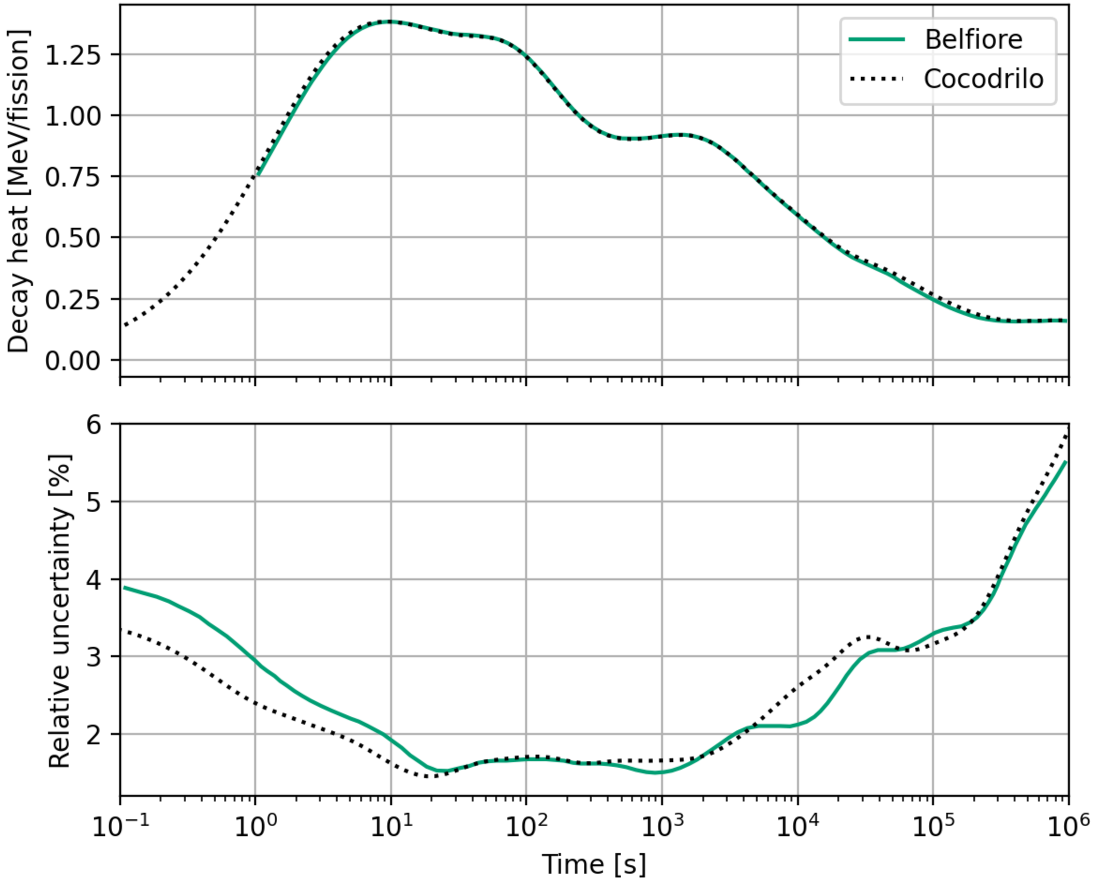
Fission yields sampling

- Study the effect of only one type of nuclear data on decay heat
- JEFF-4.0 covariance matrices available from CEA

Code-to-code comparisons

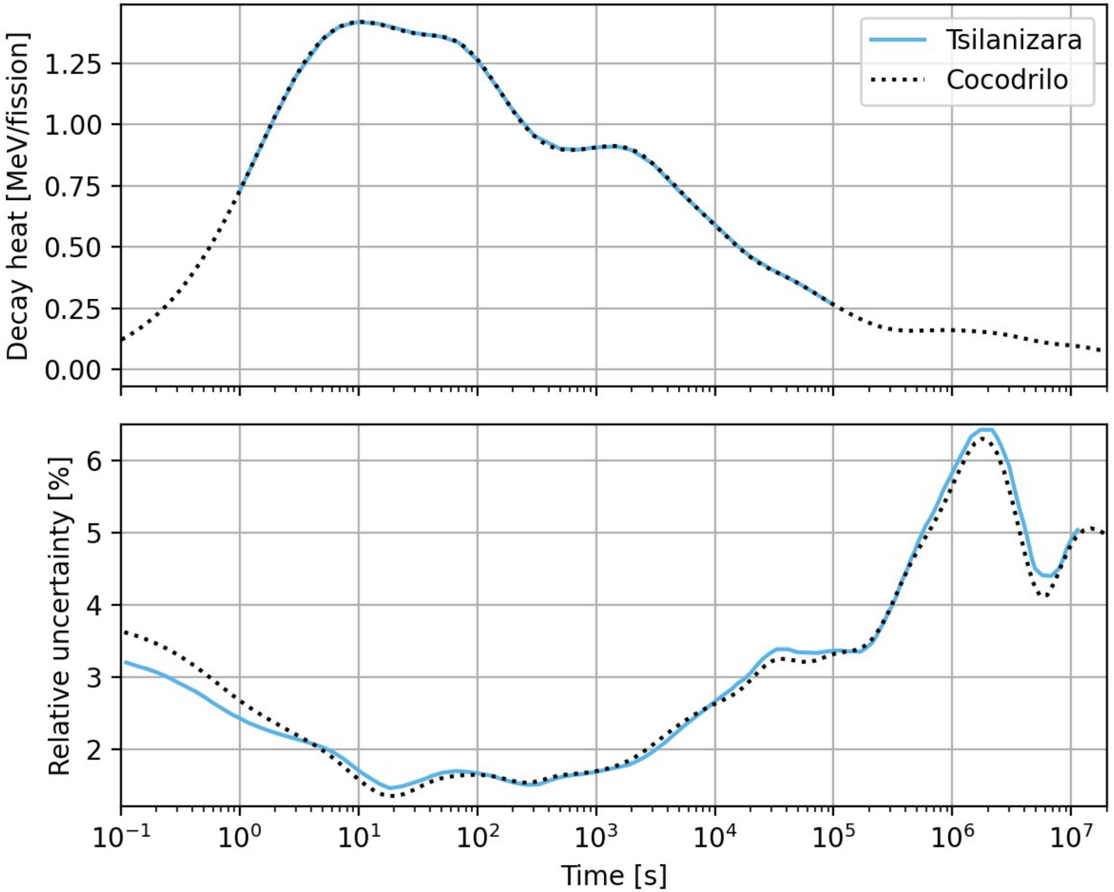
Belfiore[1]: Monte Carlo approach (SANDY code)

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



Tsilanizara[2]: S/U approach

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



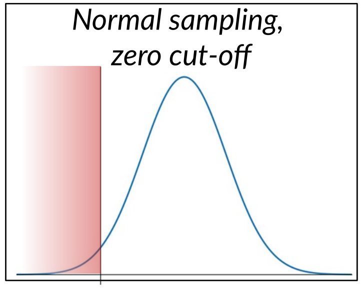
[1] E. Belfiore. "*Sensitivity and Uncertainty Analysis for Nuclear Data of Relevance in Spent Nuclear Fuel Characterization*", Master Thesis, (2023)

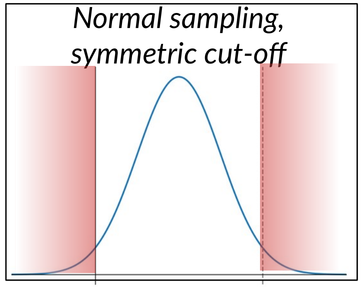
[2] A. Tsilanizara and T. Huynh. "*New feature of DARWIN/PEPIN2 inventory code: Propagation of nuclear data uncertainties to decay heat and nuclide density*". In: Annals of Nuclear Energy 164 (2021)

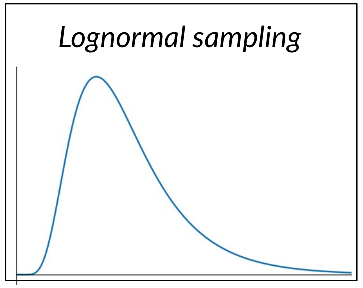
Influence of the sampling distribution

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

^{95}Nb	^{144}Pr	^{70}Cu
$\sigma/\mu = 0.34$	$\sigma/\mu = 0.58$	$\sigma/\mu = 1.59$

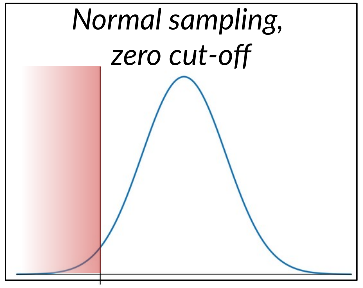


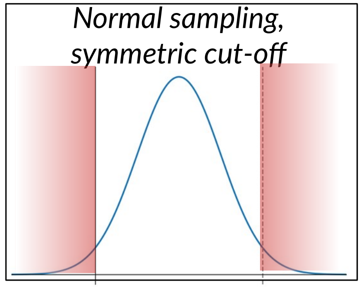


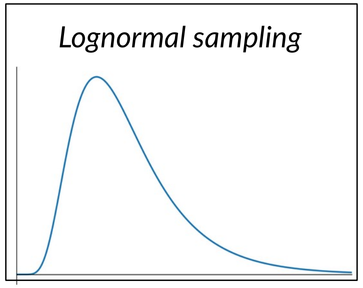


Influence of the sampling distribution

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



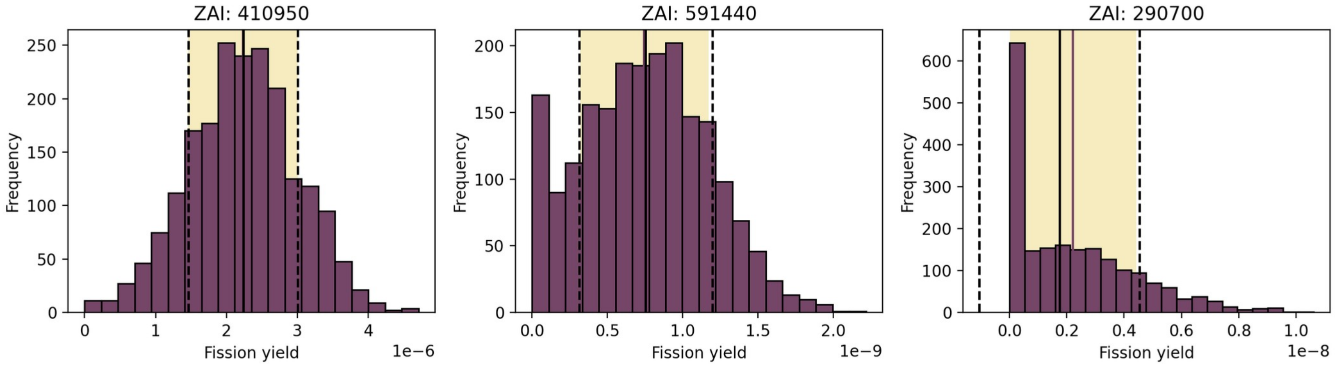




^{95}Nb $\sigma/\mu = 0.34$

^{144}Pr $\sigma/\mu = 0.58$

^{70}Cu $\sigma/\mu = 1.59$



Purple bins
Samples distribution

Purple solid line
Mean of the samples

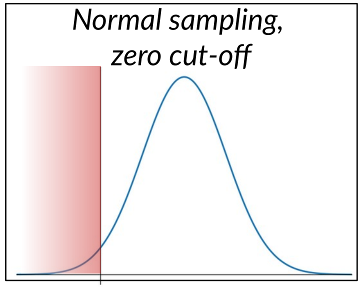
Yellow background
1 standard deviation of the samples

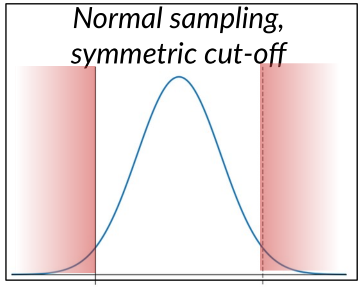
Black solid line
Reference mean

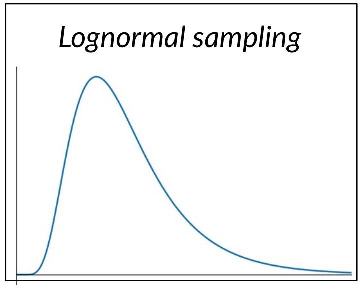
Black dashed line
Reference standard deviation

Influence of the sampling distribution

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



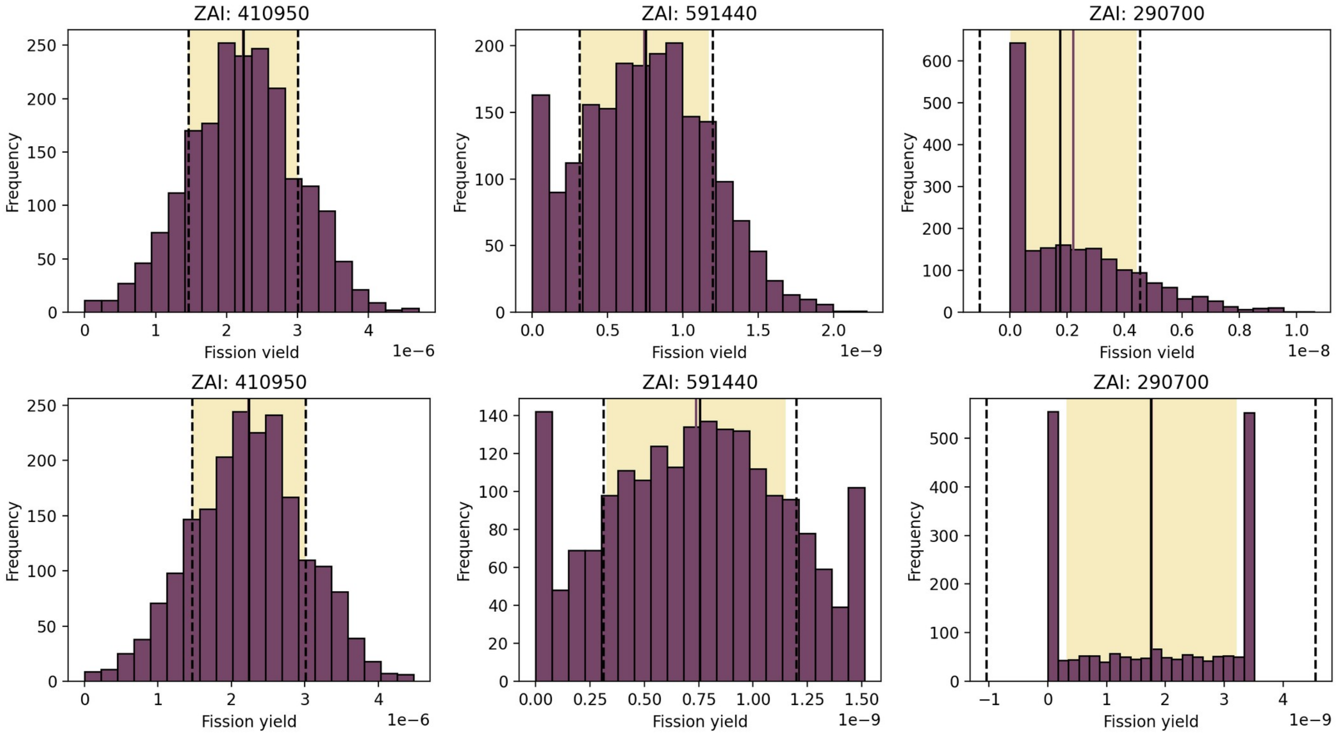




^{95}Nb $\sigma/\mu = 0.34$

^{144}Pr $\sigma/\mu = 0.58$

^{70}Cu $\sigma/\mu = 1.59$



Purple bins
Samples distribution

Purple solid line
Mean of the samples

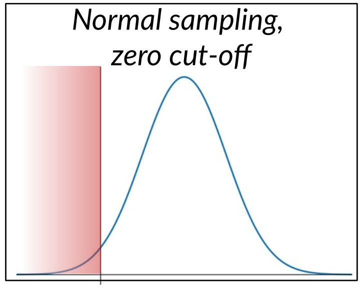
Yellow background
1 standard deviation of the samples

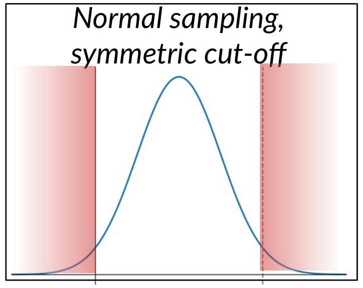
Black solid line
Reference mean

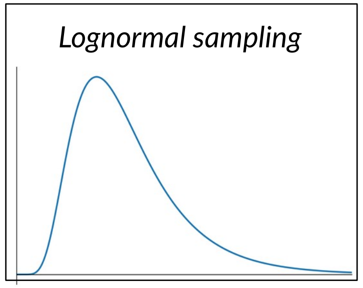
Black dashed line
Reference standard deviation

Influence of the sampling distribution

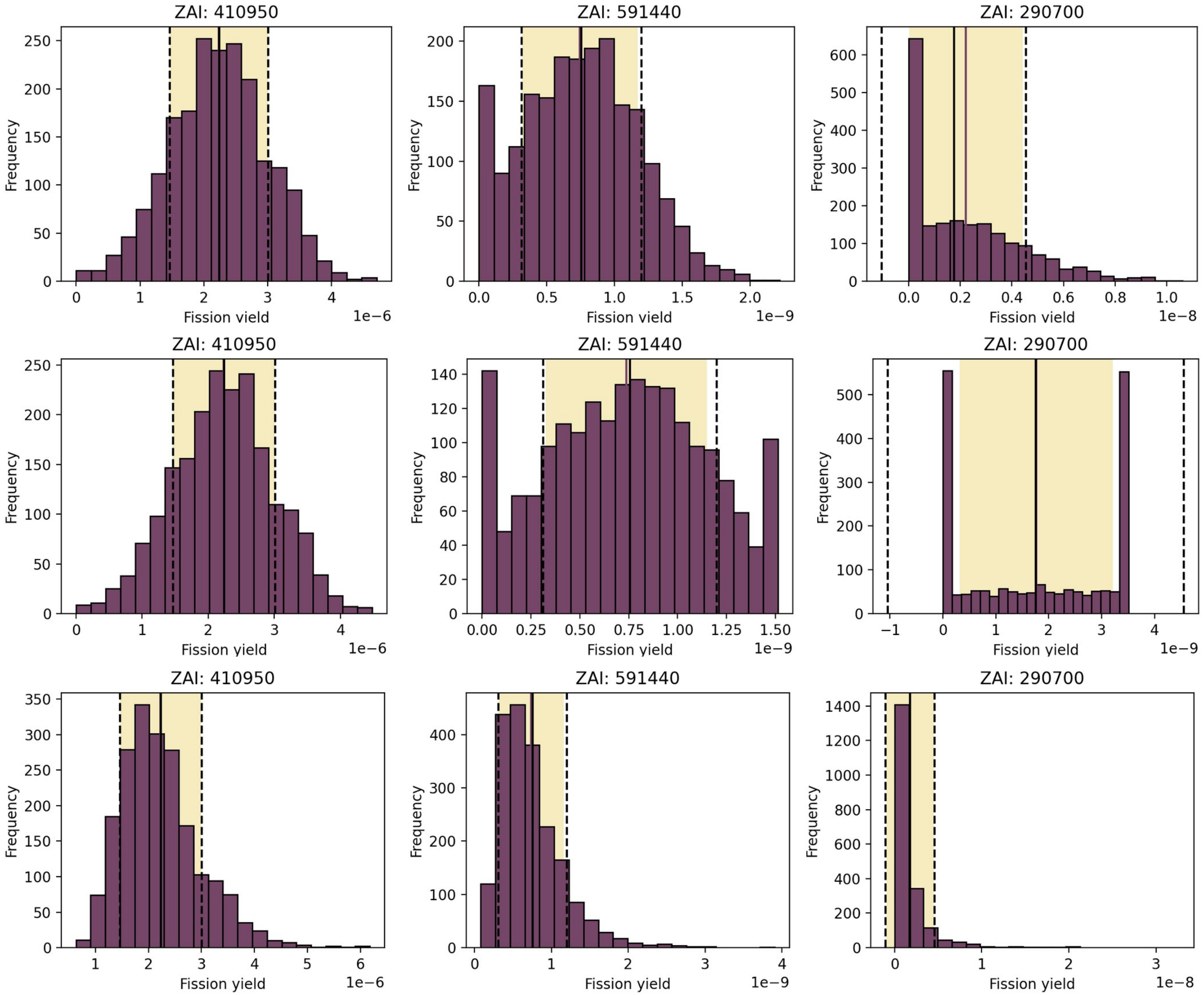
Different choices are possible on the sampling distribution and on the treatment of negative values.
Example with 2000 samples, $^{235}U_{th}$, JEFF-4.0







^{95}Nb	^{144}Pr	^{70}Cu
$\sigma/\mu = 0.34$	$\sigma/\mu = 0.58$	$\sigma/\mu = 1.59$



Purple bins
Samples distribution

Purple solid line
Mean of the samples

Yellow background
1 standard deviation of the samples

Black solid line
Reference mean

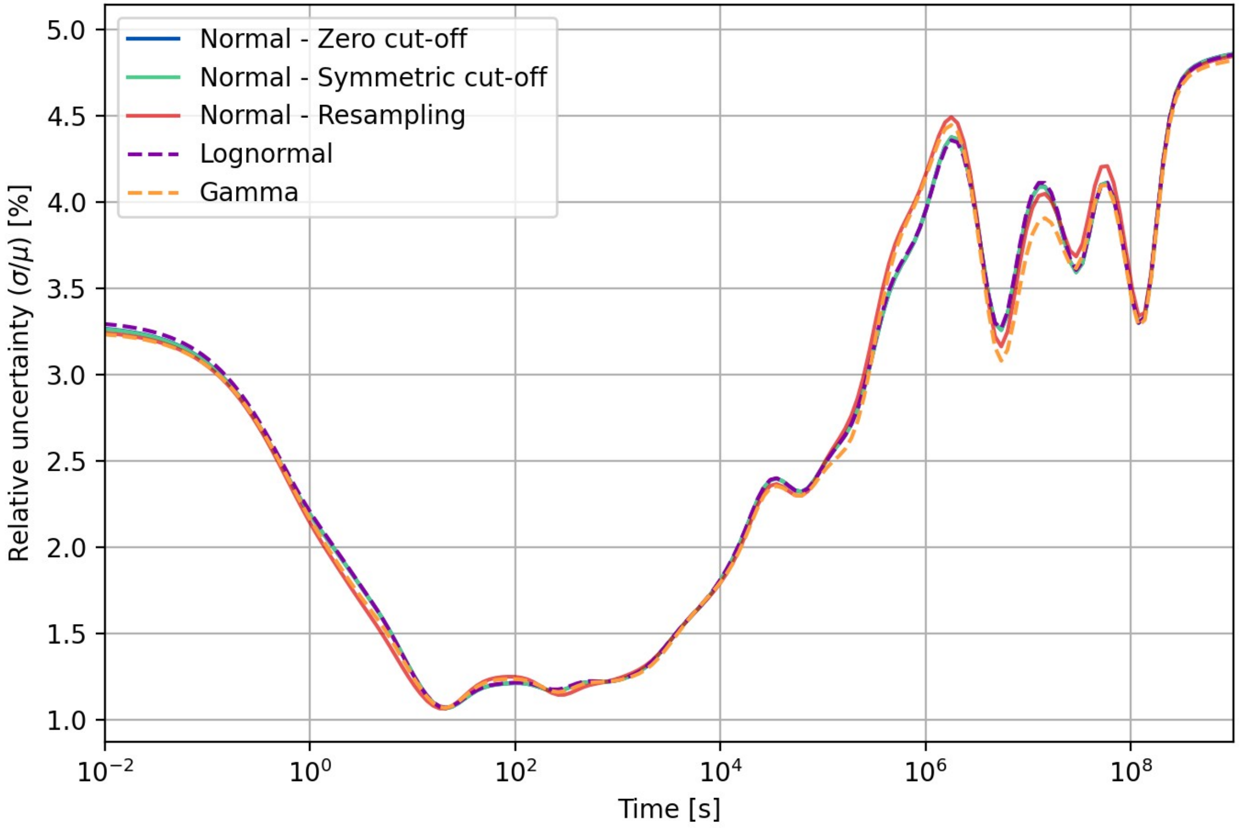
Black dashed line
Reference standard deviation

Influence of the sampling distribution

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

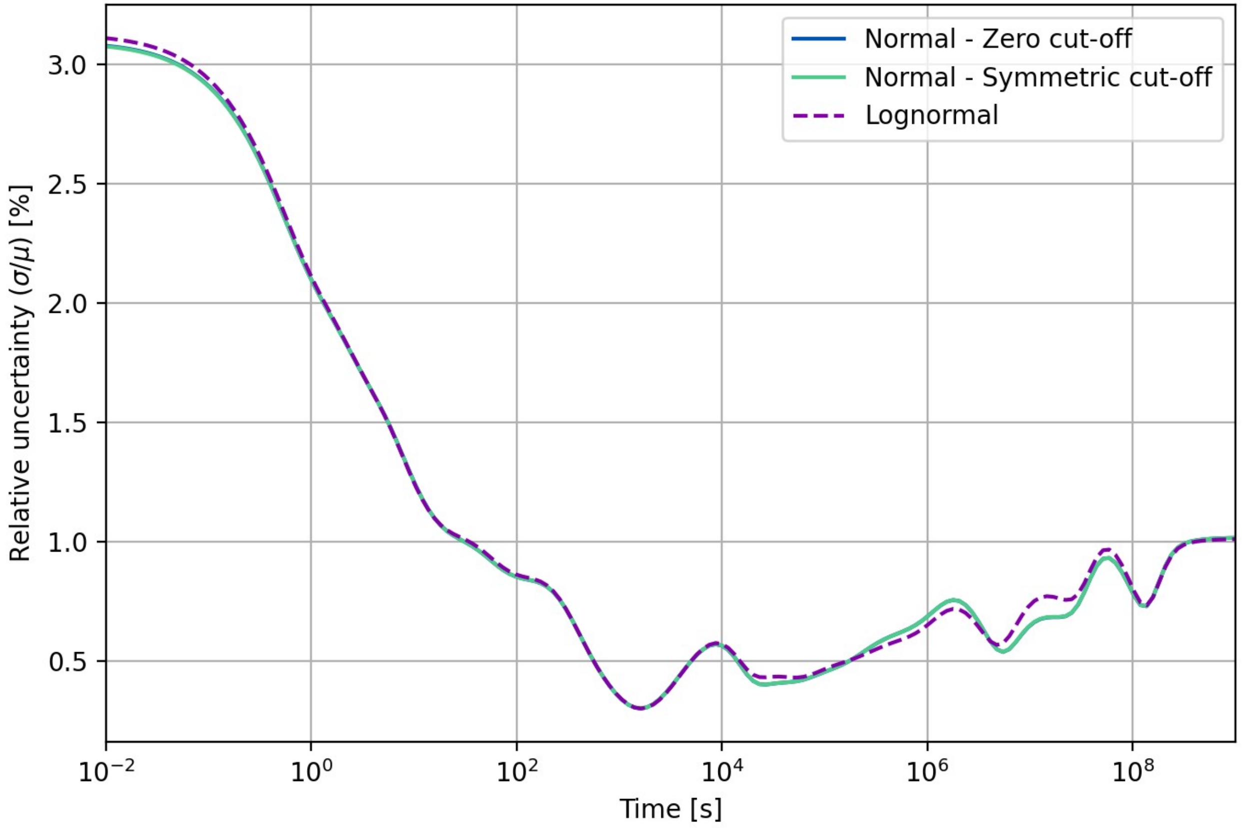
Test case: $^{235}U_{th}$ – JEFF-4.0 fission yields – 2000 samples

Without covariance matrix for fission yields



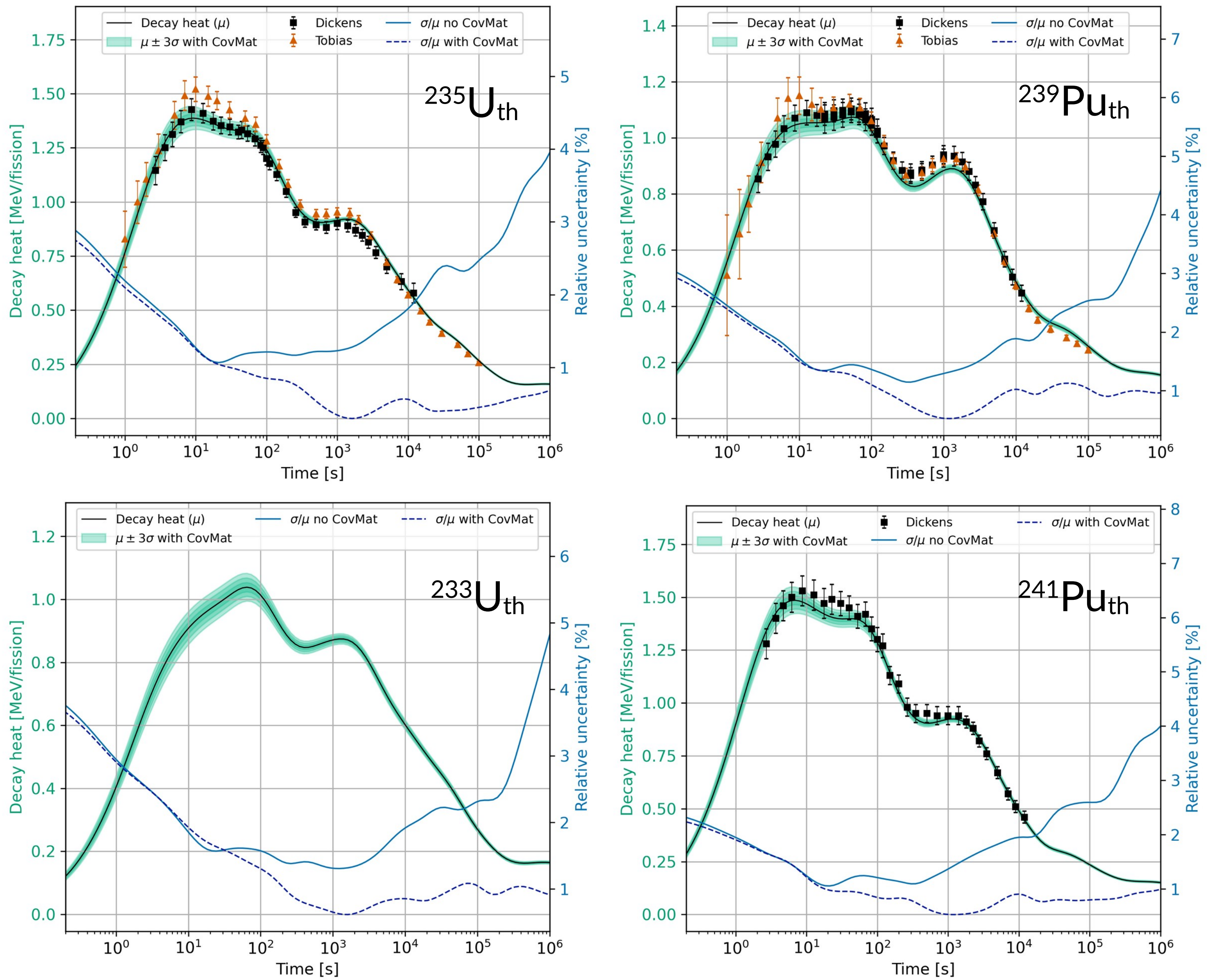
Max difference: <0.3%

With covariance matrix for fission yields



Max difference: <0.15%

JEFF-4.0 results



μ = mean value

σ = standard deviation

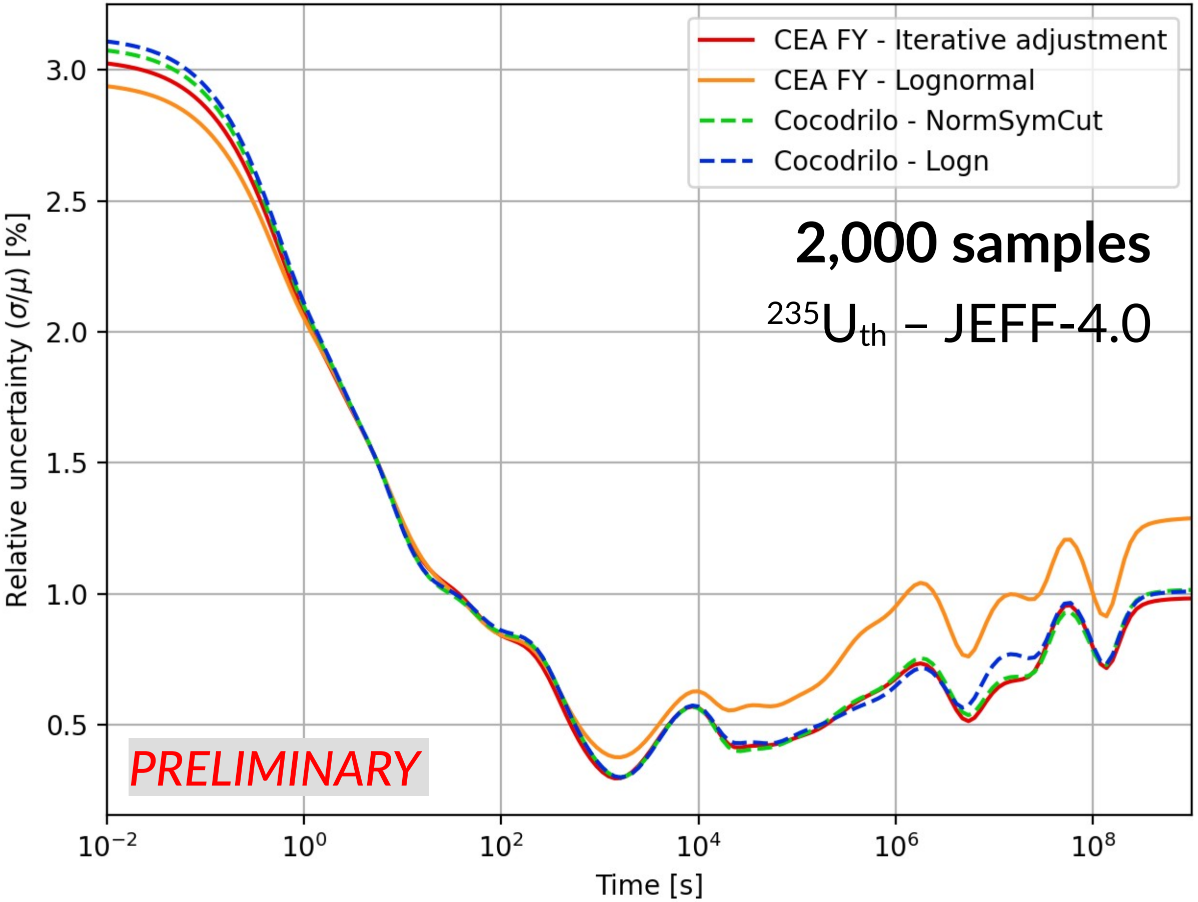
Results obtained with:

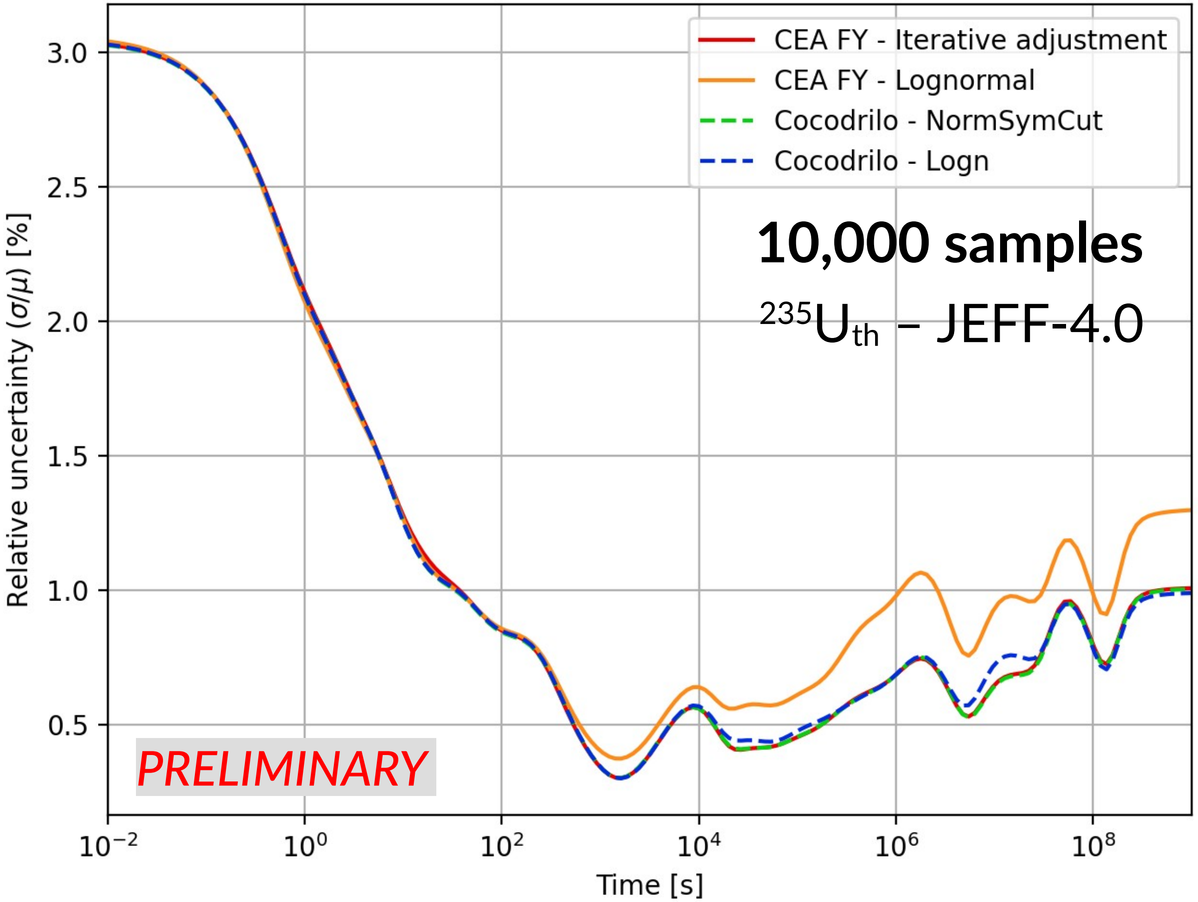
- Cocodrilo code
- Uncertainties from fission yields only
- 2000 samples
- Sampling method: Normal distribution, symmetric cut-off
- Fission Yields and covariance matrices: JEFF-4.0

+ Light particles and electromagnetic components of decay heat → back-up slides

Results using CEA's Fission Yields files

Results directly using samples generated by CEA[1]: 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 restrain on Cumulative Fission Yields.



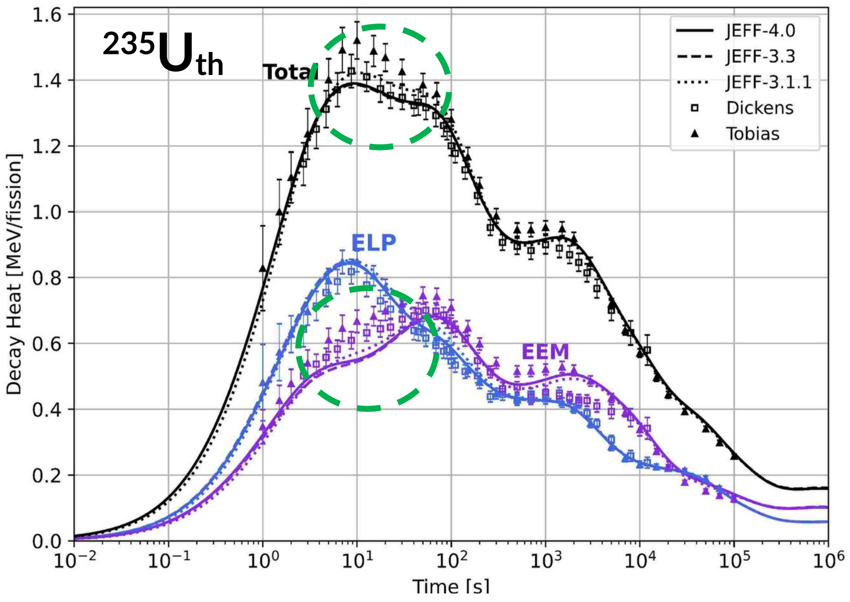


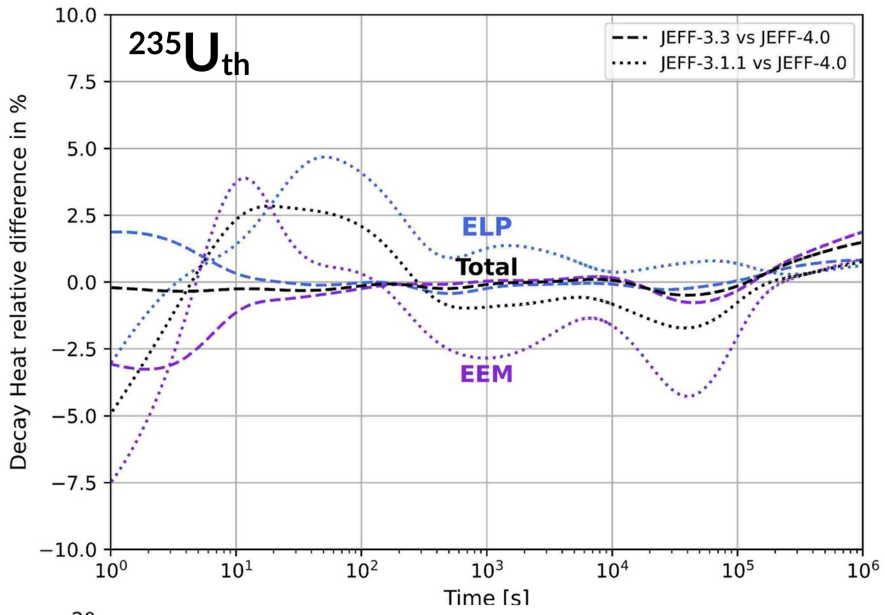
Max difference: ~0.35% for both cases

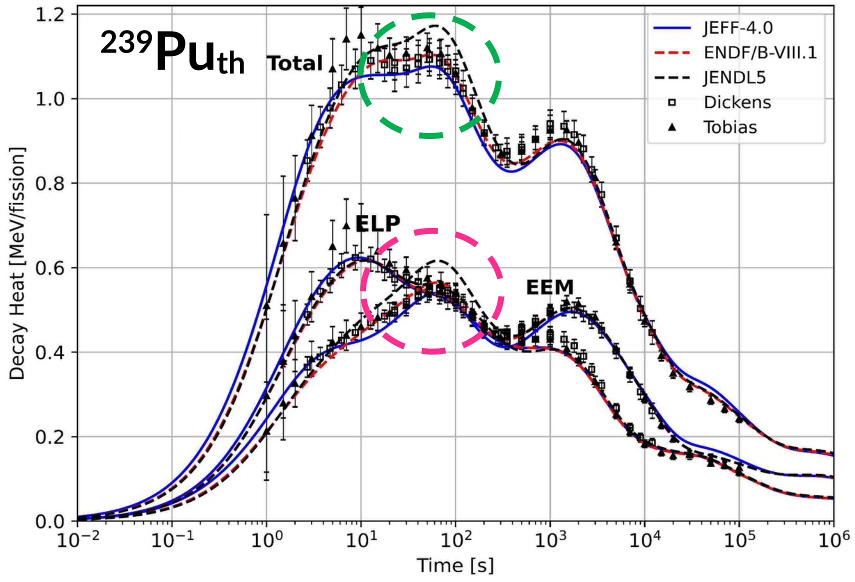
[1]G. Kessedjian et al., "*Monte Carlo Fission Yield files for the 4 major fissile nuclei*", Nuclear Data Week - JEFF meeting / APRENDE, 13-17 April 2026

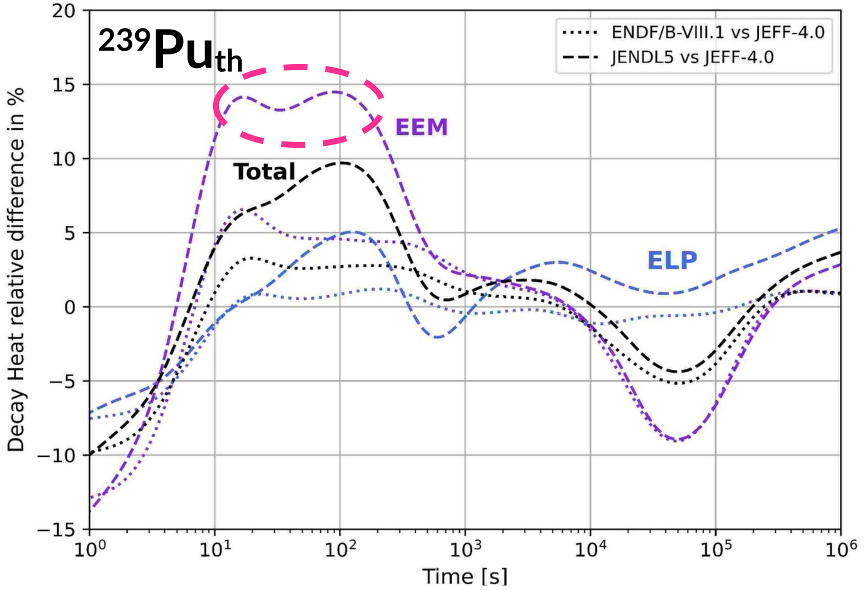
Impact of new TAGS Data in JEFF-4.0 decay data library

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









APRENDE

Total = total decay heat

ELP = Light particles component of decay heat

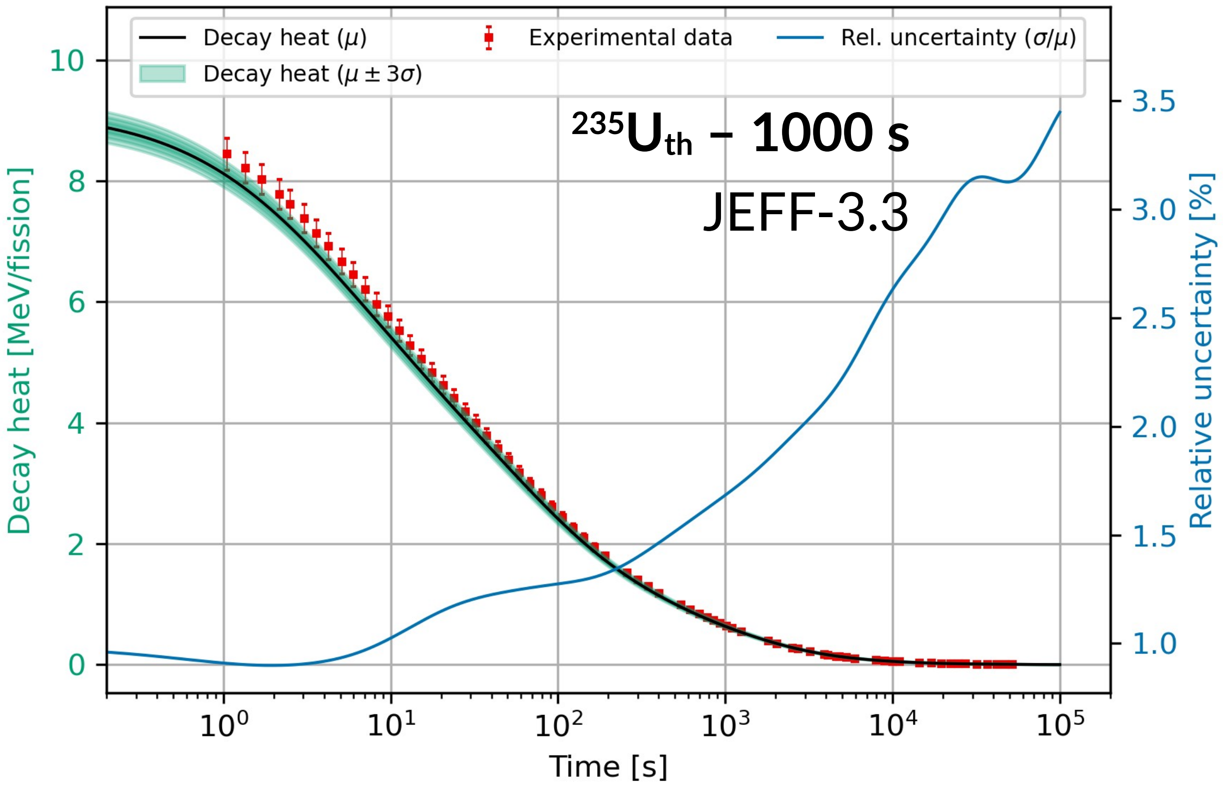
EEM = Electromagnetic component of decay heat

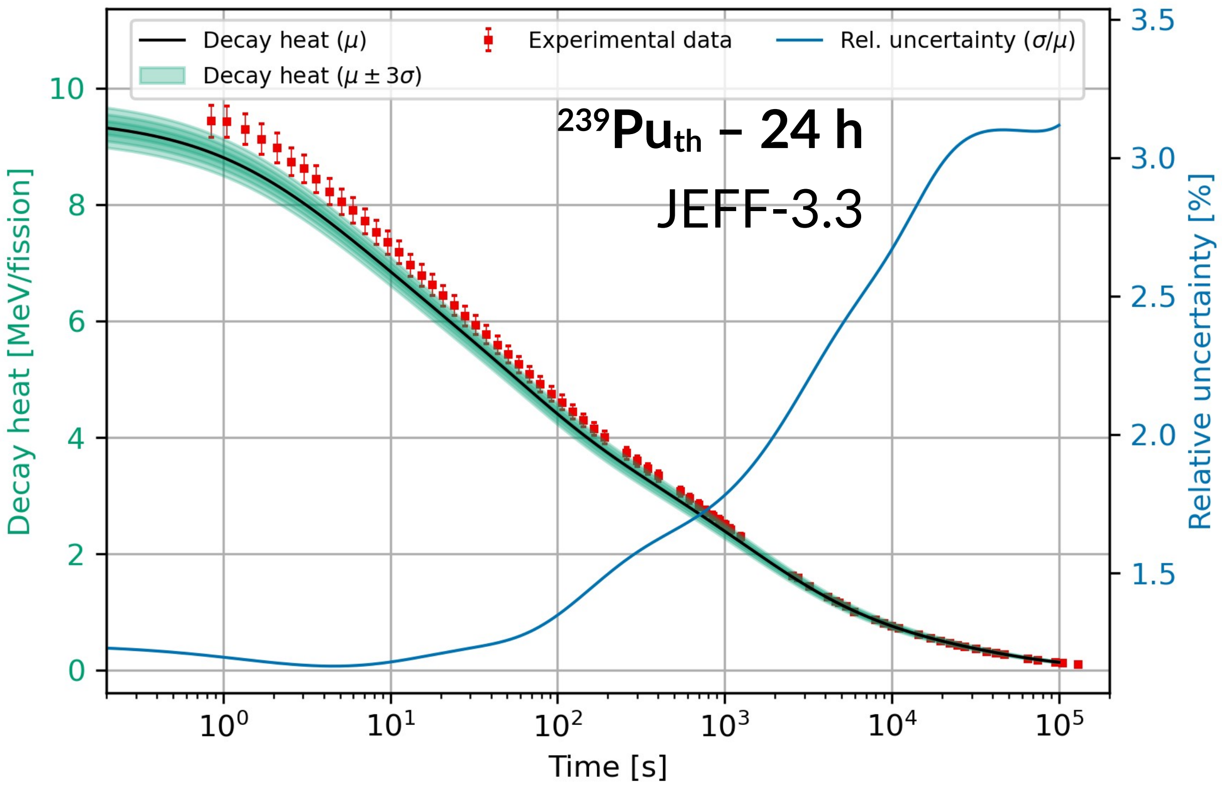
More complex cases

Longer irradiation cases: Friesenhahn et al. decay heat experiments[1,2] (1976-1979)

Experimental data available for ^{235}U (1'000s, 20'000s, 24h, 35d) and ^{239}Pu (1'000s, 24h) samples.

Results obtained sampling all FYs of JEFF-3.3 at all energies, with Normal, symmetric cut-off, no covariance matrix, 100 samples.





Possibilities to explore: influence of sampling only one or more specific **nuclides**, at one or more specific **energies**.

[1] *S. J Friesenhahn et al., 235U Fission Product Decay Heat from 1 to 105 seconds, EPRI report (1976).*

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

Conclusions and Outlooks

- Development of **Cocodrilo code** with studies on FY samplings
- **Agreement** with both MC and S/U approaches for Fission Pulses
- 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

Outlooks:

- Separate systematic uncertainty from **statistical uncertainty**
- **Decay data** sampling
- Effect of **sampling distributions** in more **complex** cases than fission pulses
- Extension of the code to **more complex cases** (assemblies and core concepts)

Thank you for your attention!

WONDER 2026

Aix-en-Provence, France

02 / 07 / 2026

Francesco Esposito

esposito@subatech.in2p3.fr

Acknowledgments

- **CNRS-IN2P3 MSR team (LPSC-Grenoble, Subatech):** Michel Allibert, Lydie Giot, Daniel Heuer, Axel Laureau, Elsa Merle

  on this topic :
  PhD students: Jad Halwani, Yohannes Molla
  and interns: Florent Hervy, David Laks

- Support of **Master Project/DONEE** (CNRS)

- **Aprende European project** (Addressing PRiorities of Evaluated Nuclear Data in Europe), European Union's HORIZON-EURATOM under grant agreement No. 101164596

  Collaboration with Sofia Portolan (PSI, EPFL), Dimitri Rochman (NAGRA)

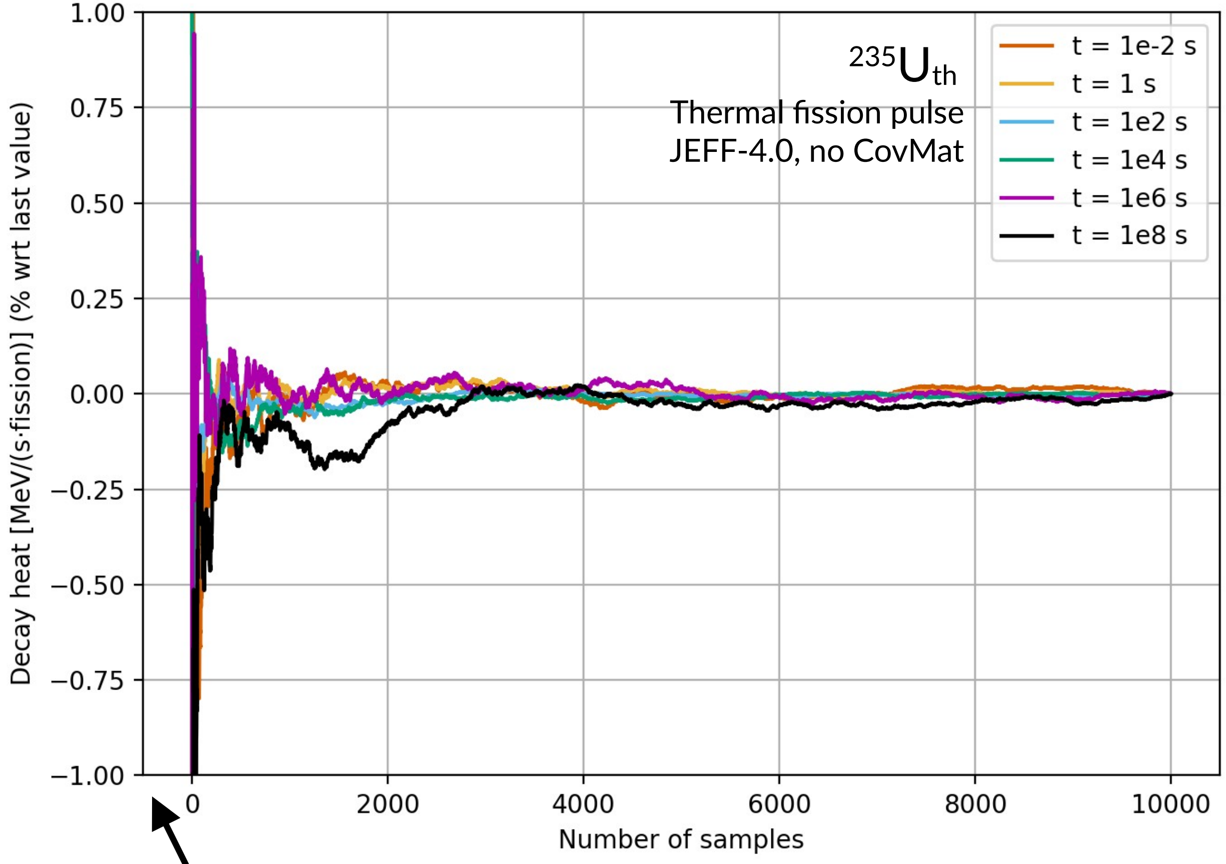
  Collaboration with Fanny Farget (GANIL), Diego Ramos (GANIL)

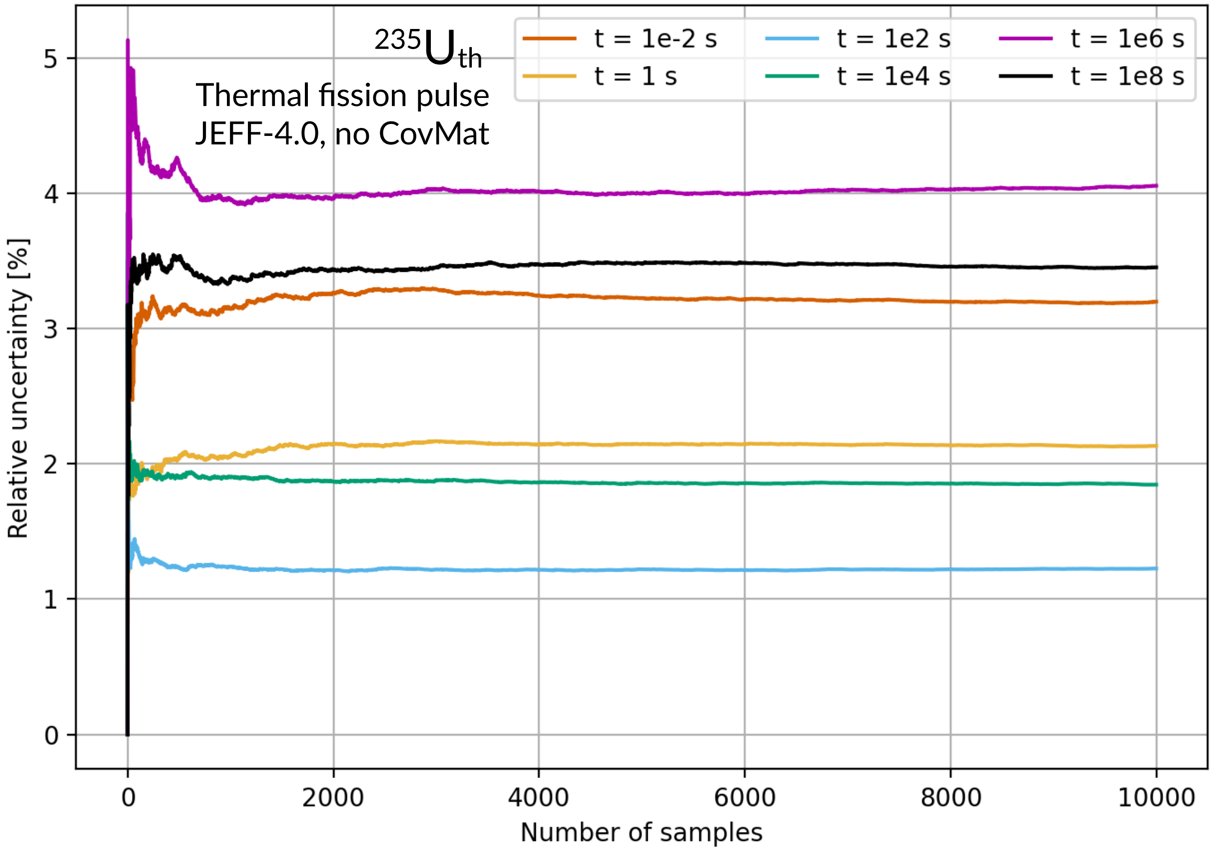
- **ENDURANCE European project** (EU kNowleDge hUb foR enabling MolteN Salt ReaCtor safety development and DEployment), European Union's HORIZON-EURATOM under grant agreement No. 101164596, mobility grants.

- **TAS collaboration** (IFIC Valencia, SEN team@Subatech, Univ. of Surrey) for providing TAGS data and scientific discussions

Backup – Effect of the number of samples

Convergence of mean value and of relative uncertainty at fixed cooling times

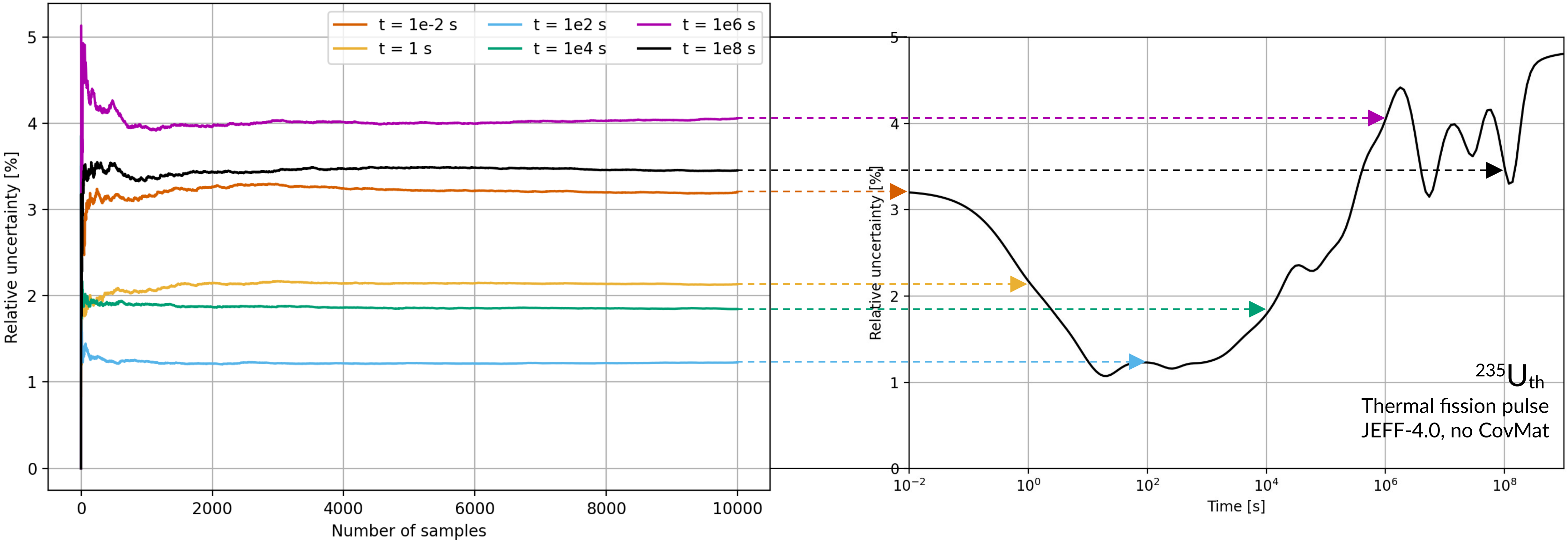




1% (not 100%)

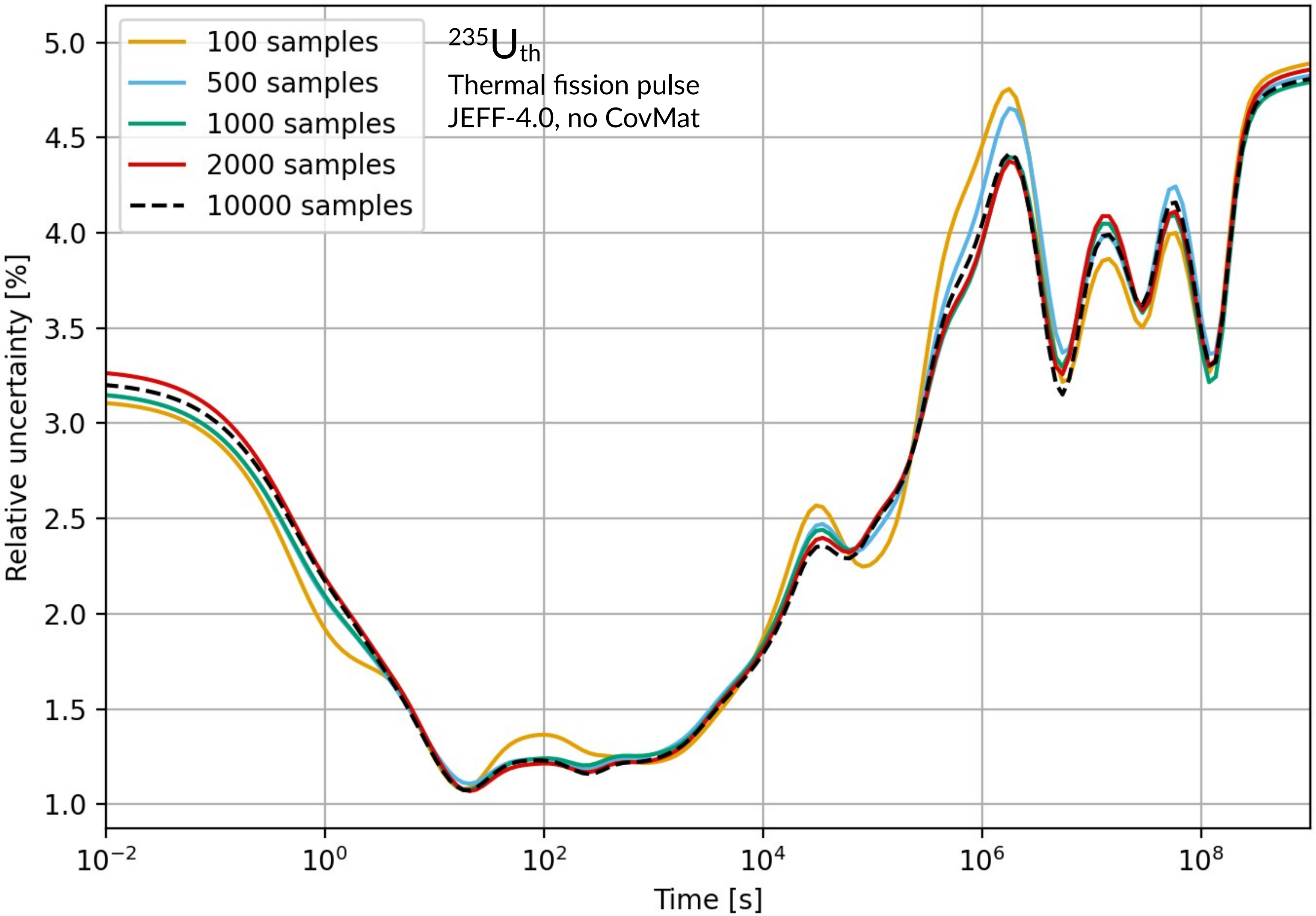
Backup – Effect of the number of samples

Correspondence of converged relative uncertainty on the full profile

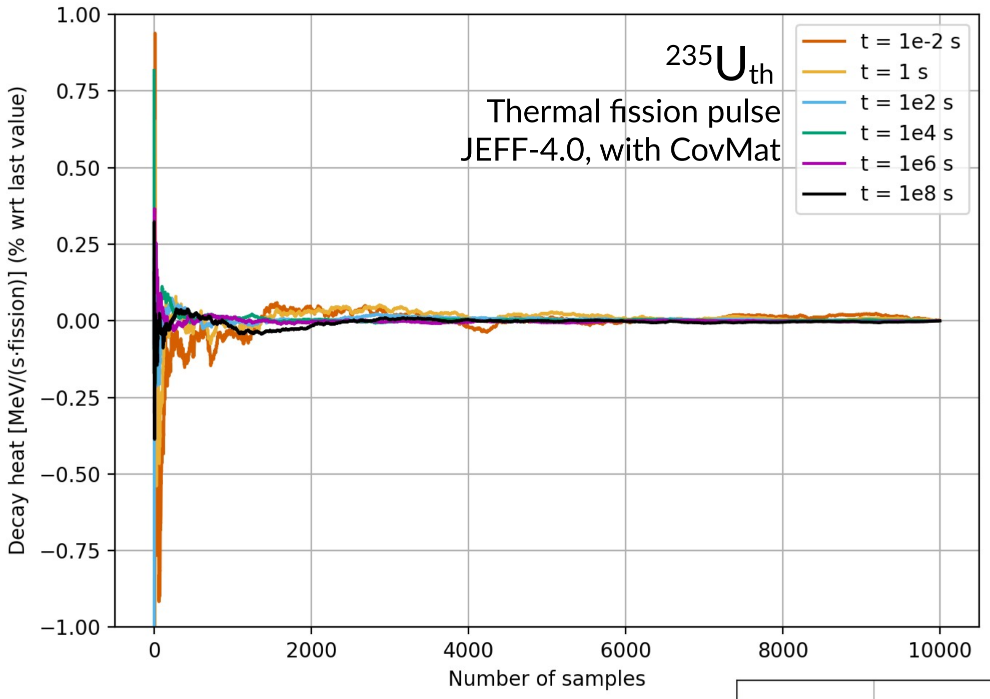


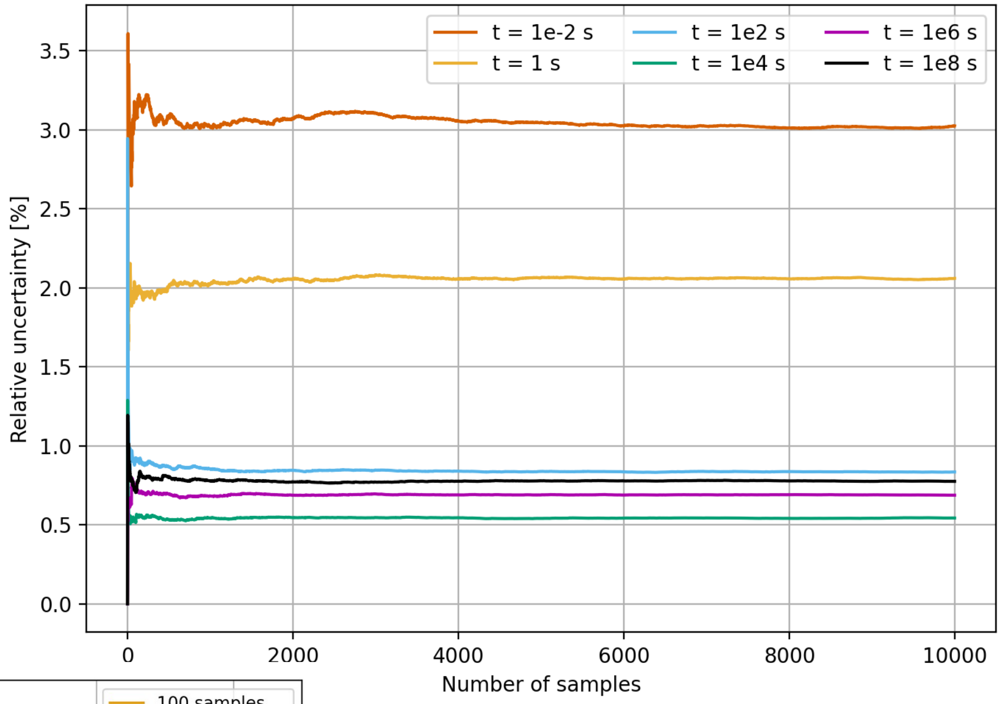
Backup – Effect of the number of samples

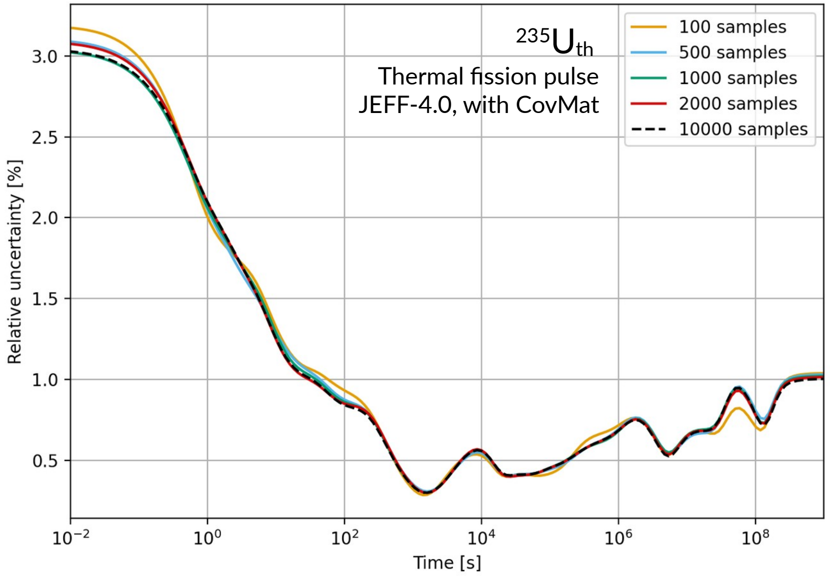
Evolution of relative uncertainty curve at different number of samples



Backup – Effect of the number of samples





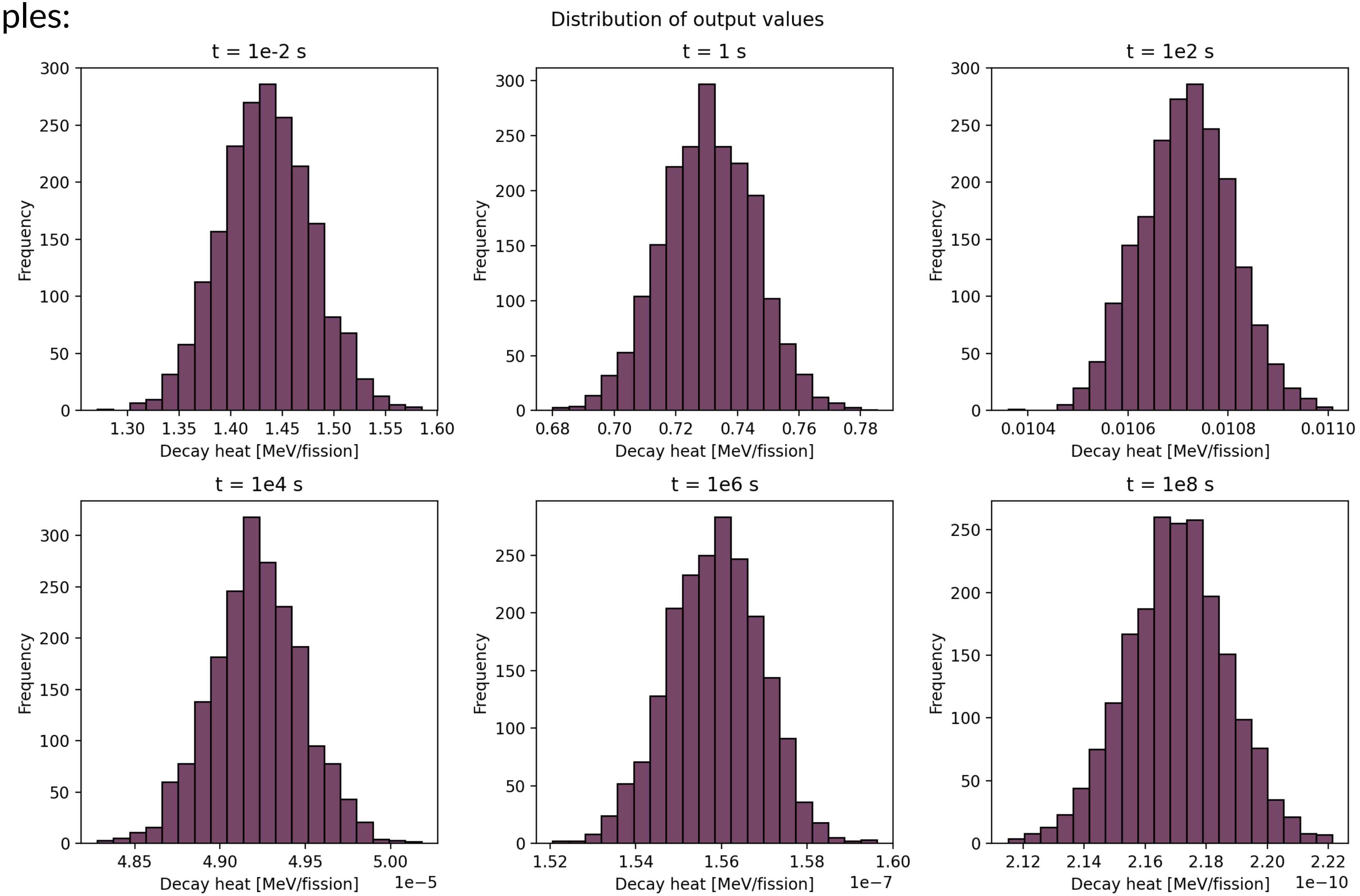


With covariance matrix, results seem to converge faster

Backup – Distribution of output values

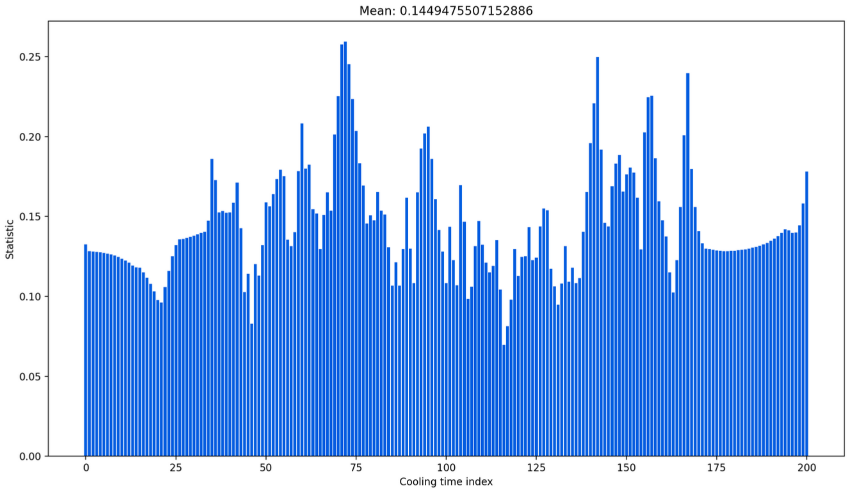
After 2000 samples:

$^{235}U_{th}$
Thermal fission pulse
JEFF-4.0, no CovMat

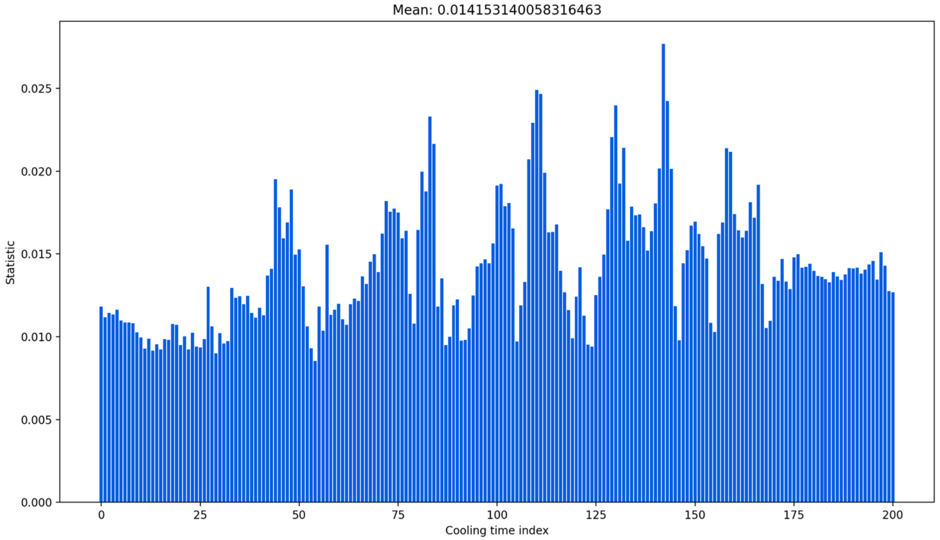


Backup – Distribution of output values – KS statistic

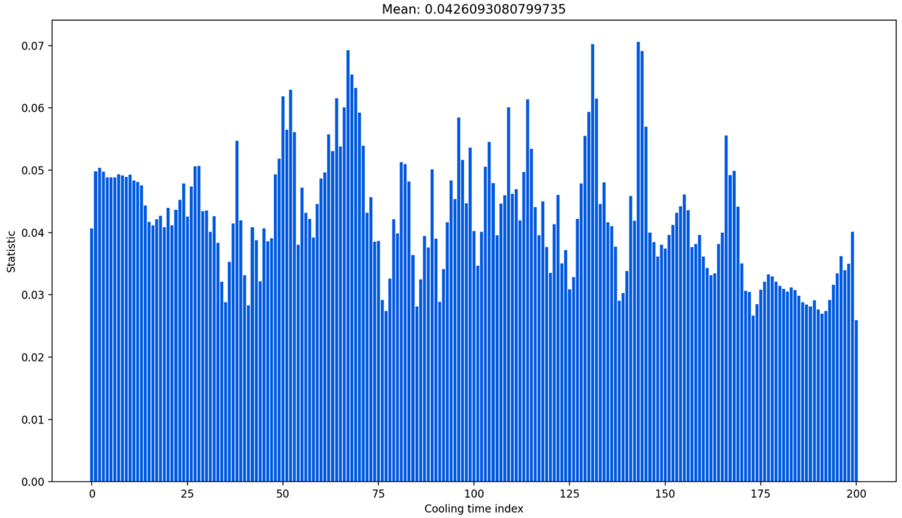
20 samples – Mean: **0.15**



2000 samples – Mean: **0.014**



200 samples – Mean: **0.042**



Kolmogorov-Smirnov statistic

$^{235}U_{th}$

Thermal fission pulse

JEFF-4.0, no CovMat

Backup – Procedure used by CEA for sampling FY

SetZero

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

- spectral decomposition

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

- Sampling

$\boldsymbol{S} \rightarrow \mathcal{N}(\mathbf{0},\mathbf{I_n})$

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

- Regularization

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

LogNormal

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

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

- Regularization

$Arg > 0$ $Arg < 0$

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

$Corr_{ij}$

- Sampling

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

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

$\boldsymbol{S} \rightarrow \mathcal{N}(\mathbf{0},\mathbf{I_n})$

$y_{s,i} = exp\left(\mathrm{y}_{s,i}^{\mathrm{LN}}\right)$

iterative adjustment

- *Cholesky decomposition*

Find L : $\mathbf{Cov_Y} = \mathbf{LL^T}$

- Sampling

$\boldsymbol{S} \rightarrow \mathcal{N}(\mathbf{0},\mathbf{I_n})$

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

- Regularization

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

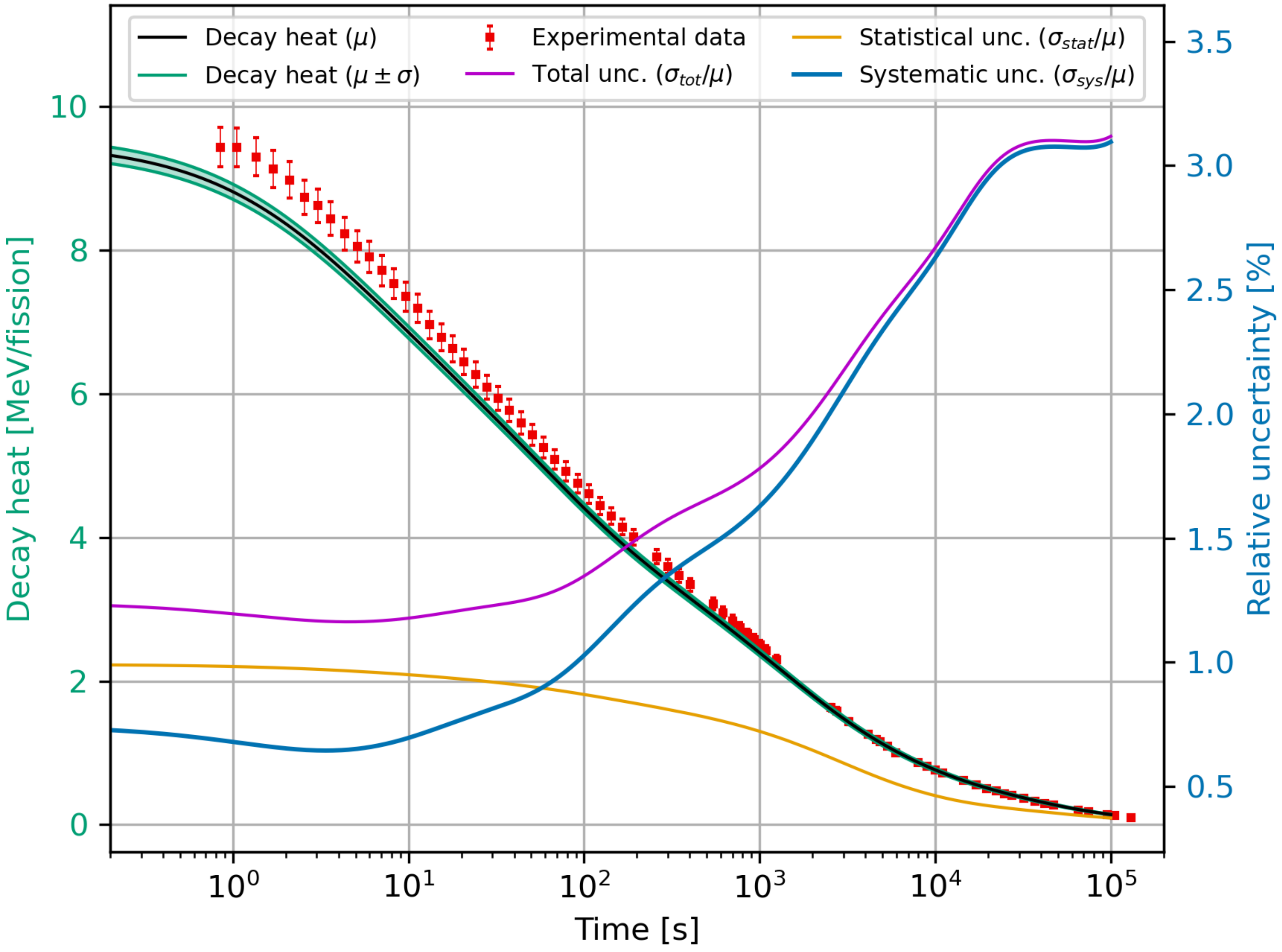
- k Iterative process

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

cea G. Kessedjian et al. - Nuclear Data Week - JEFF meeting / APRENDE, 13-17 April 2026 8

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

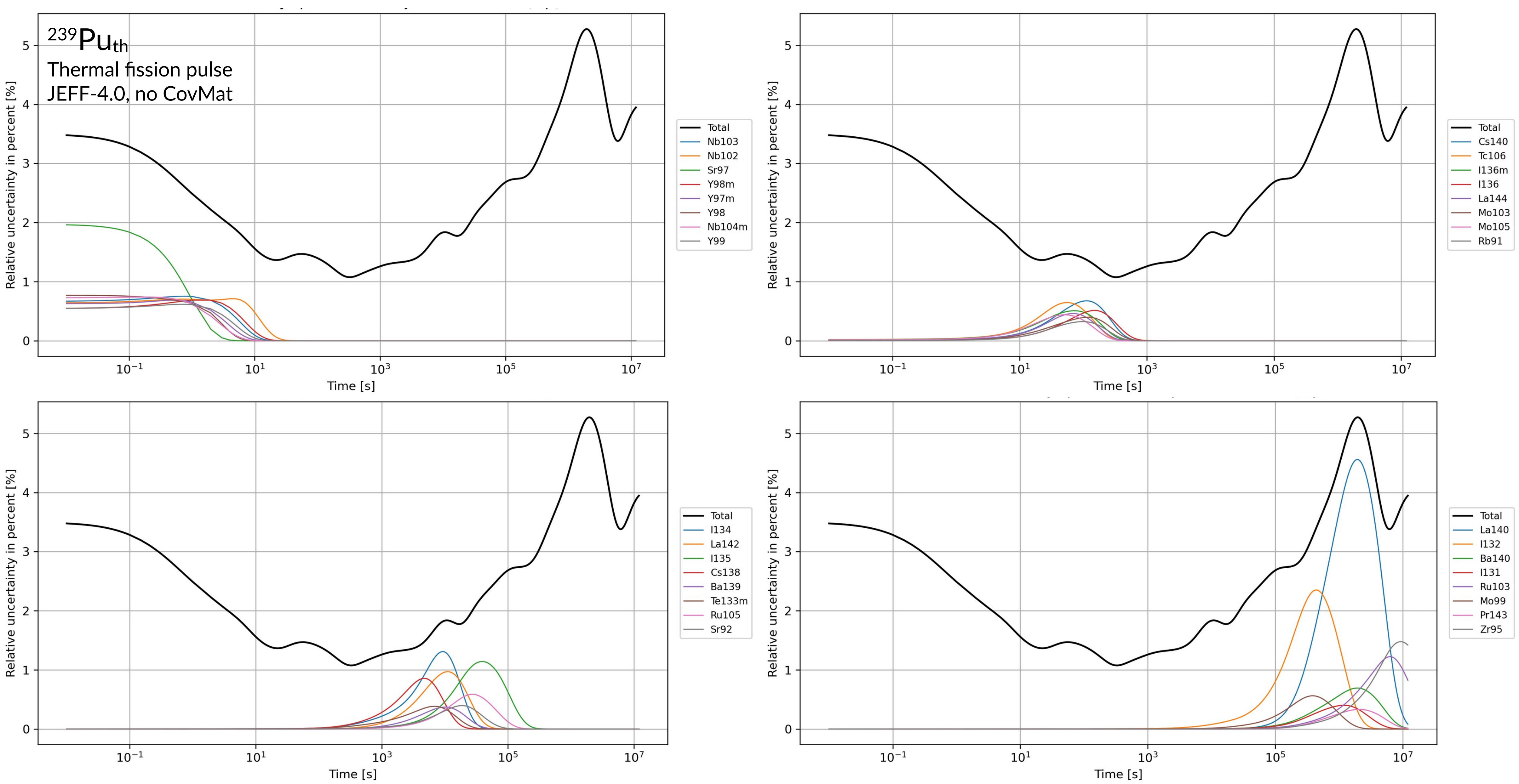
Backup – Statistical uncertainty



- Friesenhahn setup
- $^{239}Pu_{th}$, 24h irradiation
- Cocodrilo code
- Uncertainties from fission yields only
- 100 samples
- Sampling method: normal with symmetric cut-off, no covariance matrix
- JEFF-3.1.1
- Statistical uncertainty calculated with 100 fixed samples (“virtual samples”)

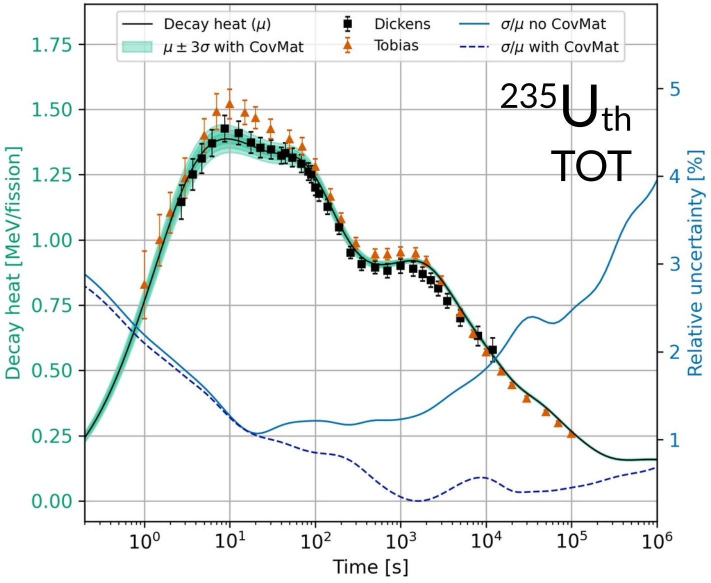
$$\sigma_{sys} = \sqrt{\sigma_{tot}^2 - \sigma_{stat}^2}$$

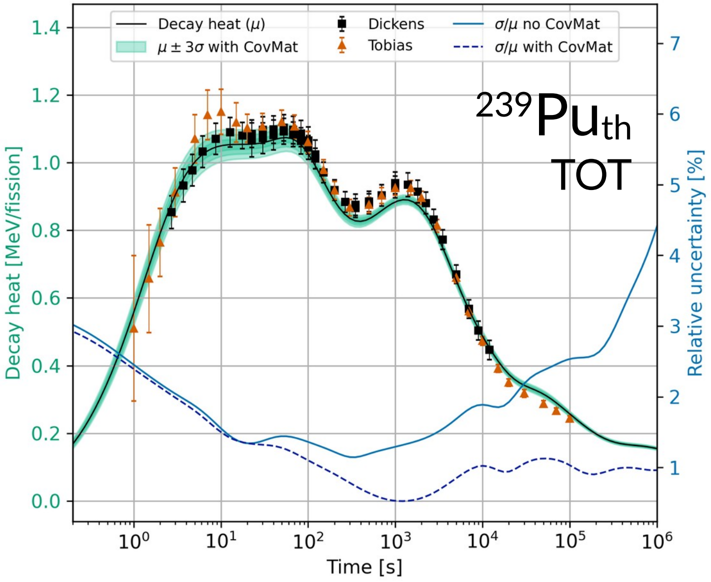
Backup – Contribution of nuclides to uncertainty



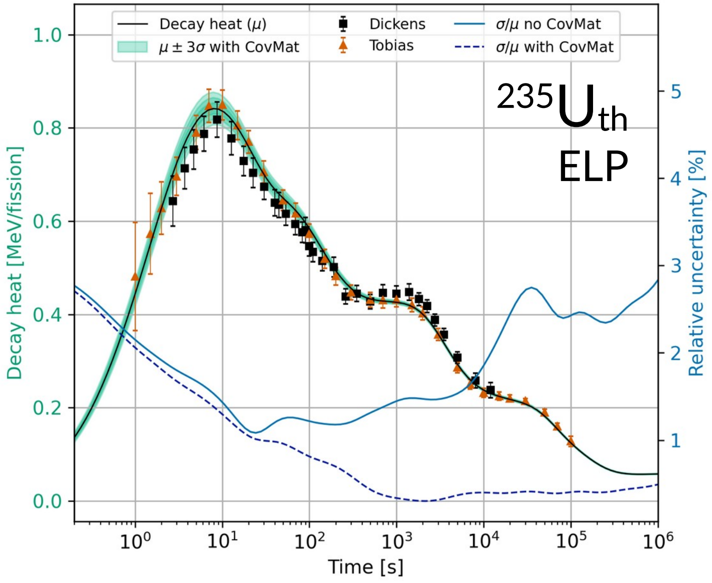
Other JEFF-4.0 results

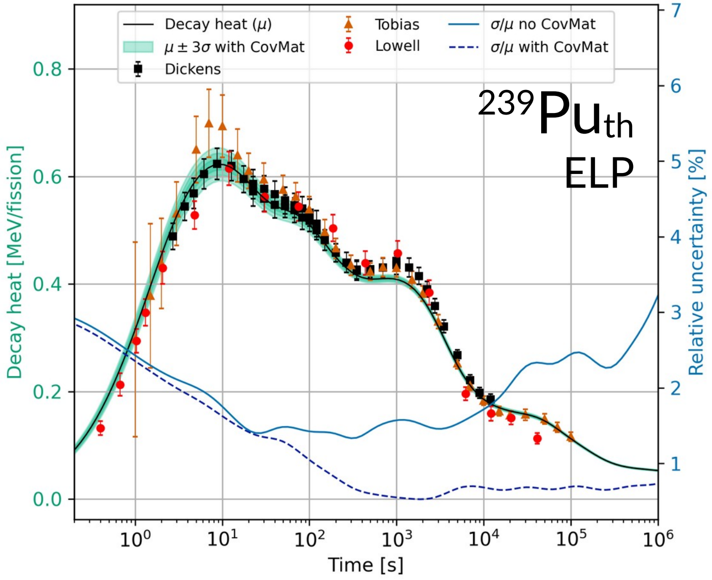
Total decay heat



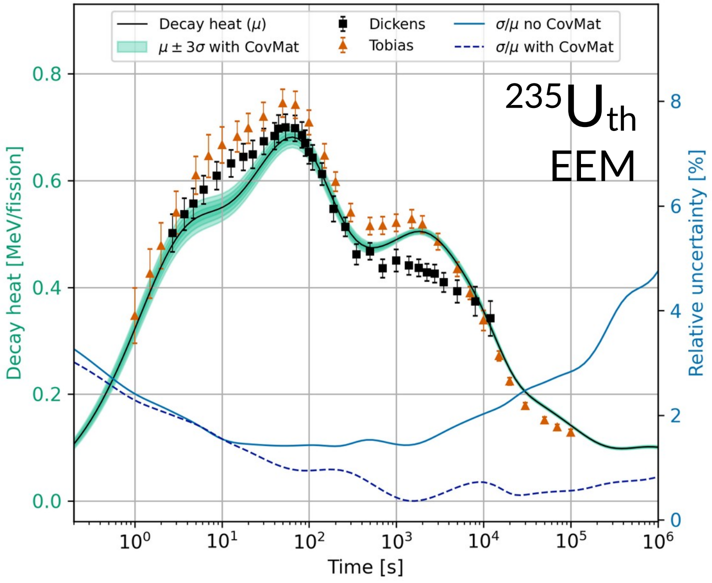


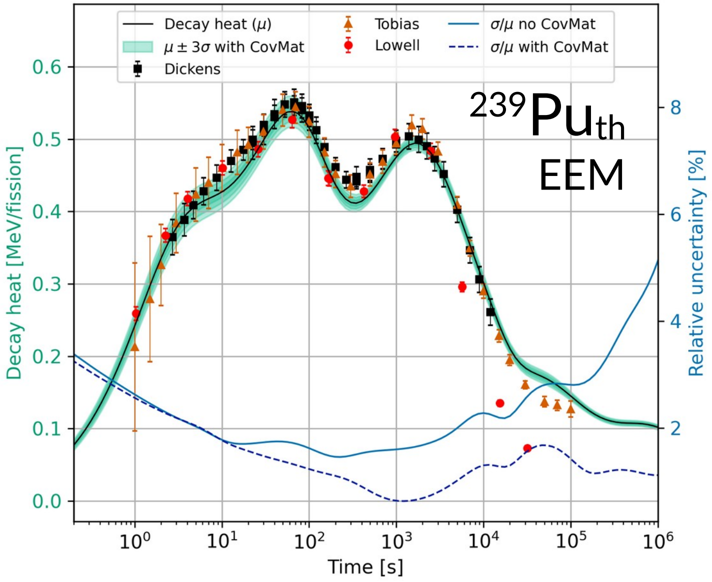
Light particles component





Electromagnetic component



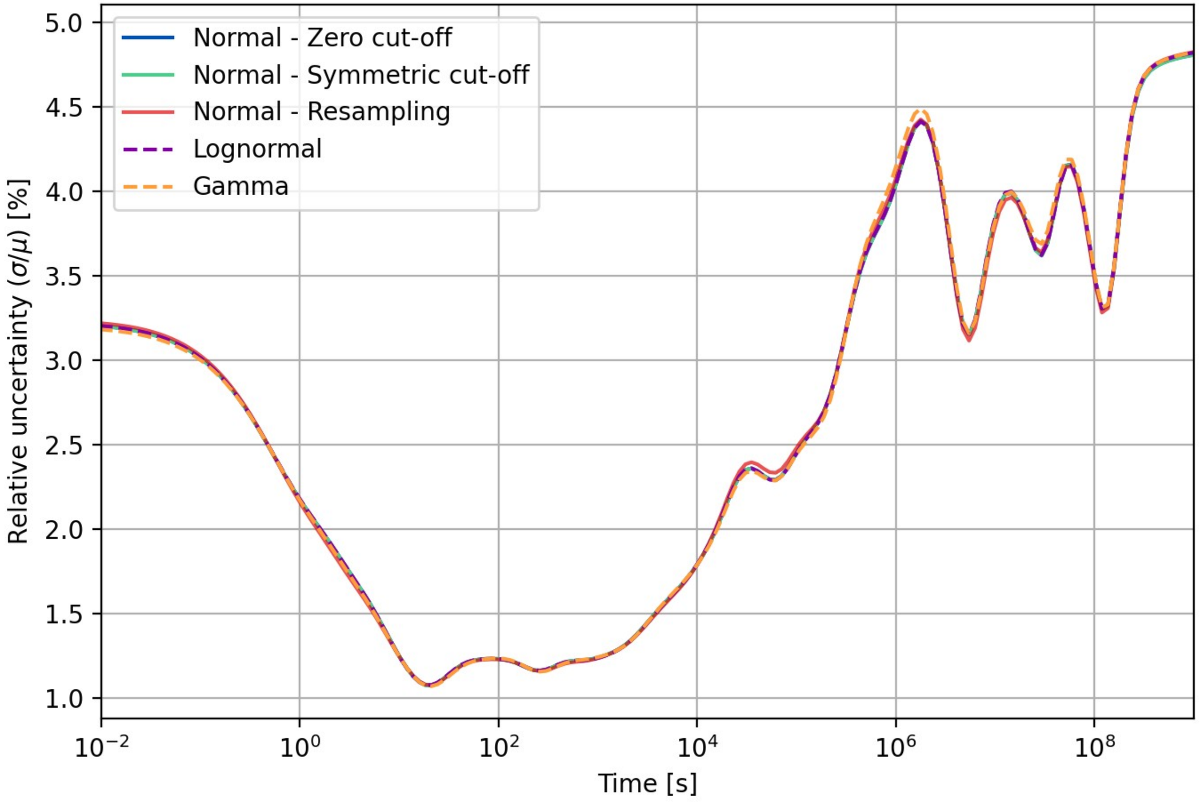


Influence of the sampling distribution

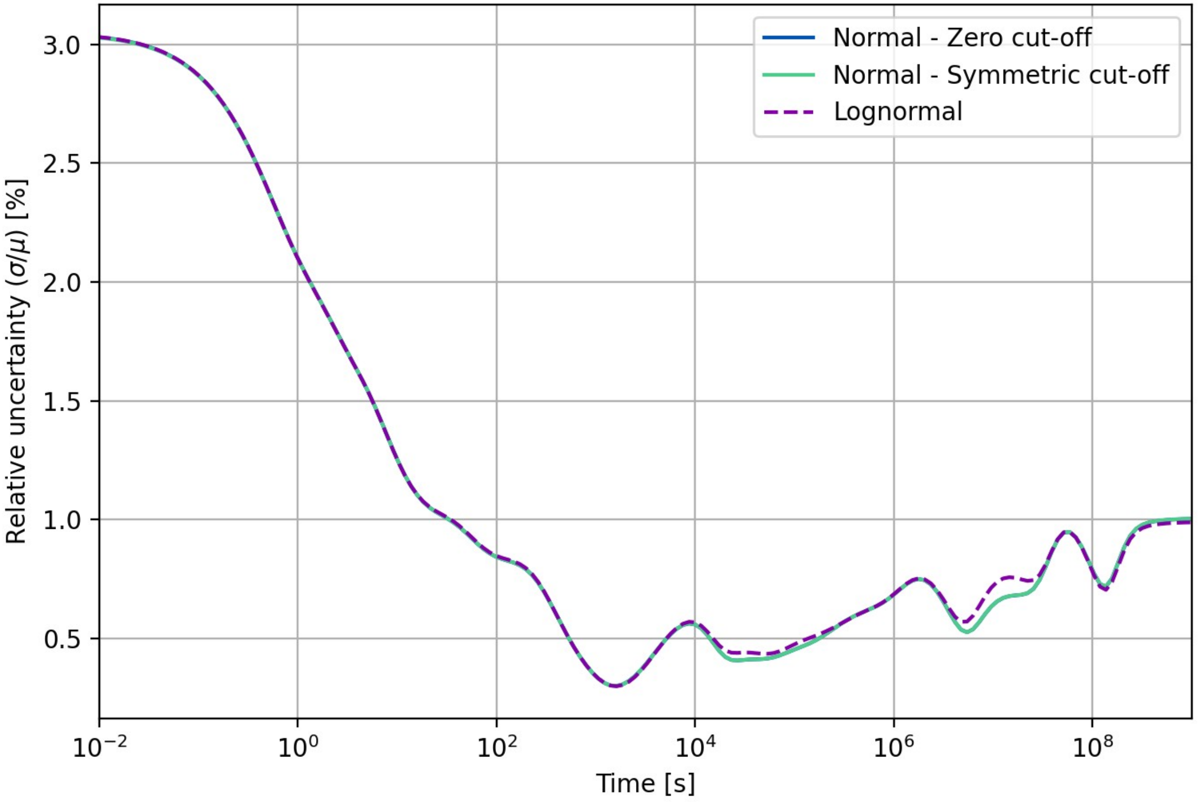
With more samples, the effect of the sampling distribution is even smaller

Test case: $^{235}U_{th}$ – JEFF-4.0 fission yields – **10'000** samples

Without covariance matrix for fission yields



With covariance matrix for fission yields



To be compared with slide 7

Backup – Indicators for samples quality

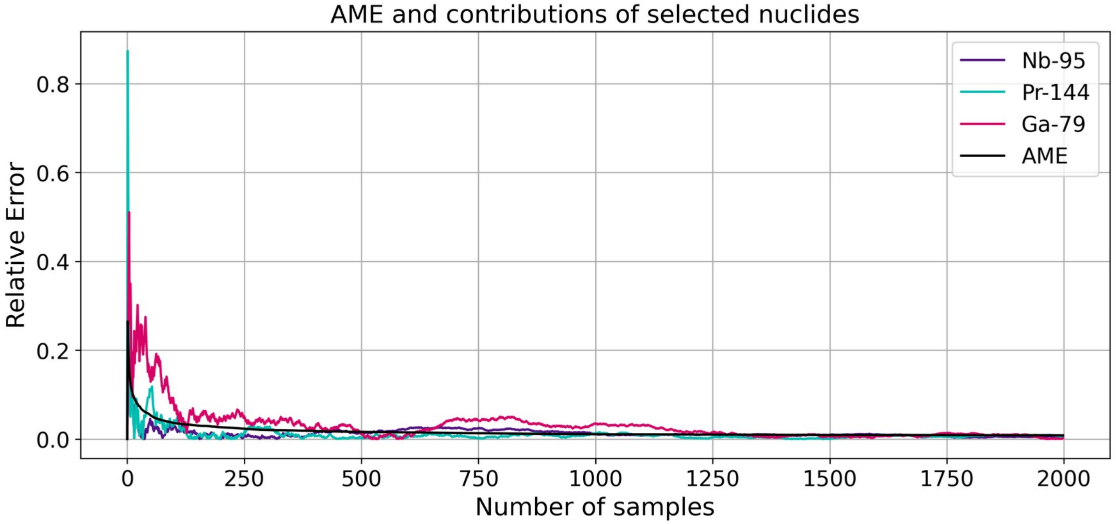
How many nuclides are affected by such distorted distributions?

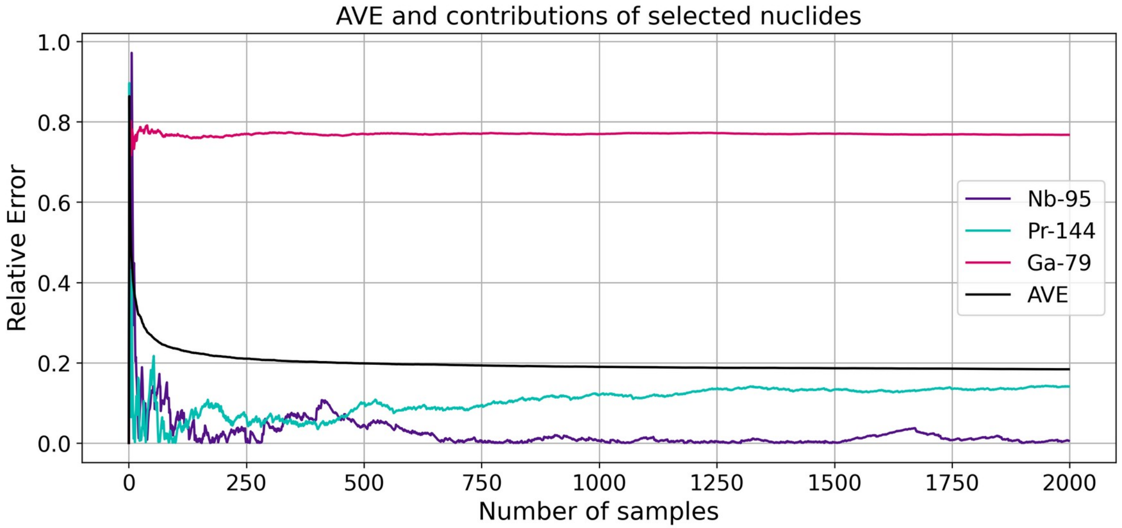
- Application of indicators found in literature
- Development of new indicators to have a clearer view

$$\mathrm{AME}(N) = \frac{1}{M}\sum_{i=1}^{M} \mathrm{ME}_i(N) = \frac{1}{M}\sum_{i=1}^{M}\left|\frac{m_i(N)}{\mu_i} - 1\right|$$

$$\mathrm{AVE}(N) = \frac{1}{M}\sum_{i=1}^{M} \mathrm{VE}_i(N) = \frac{1}{M}\sum_{i=1}^{M}\left|\frac{s_i^2(N)}{\sigma_i^2} - 1\right|$$

Example with 2000 samples from JEFF-4.0, fission yields of $^{239}Pu_{th}$, Normal symmetric cut-off:

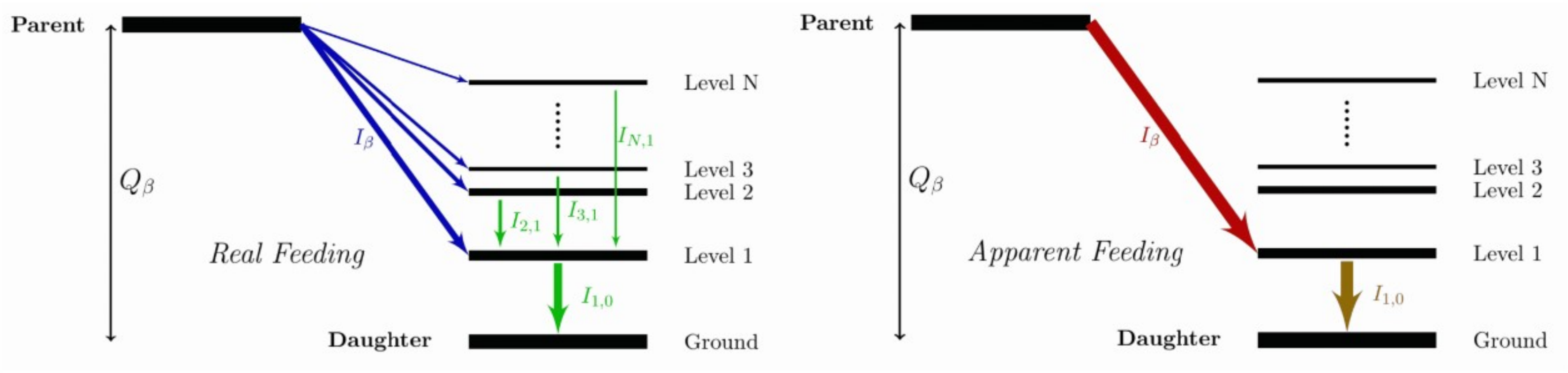




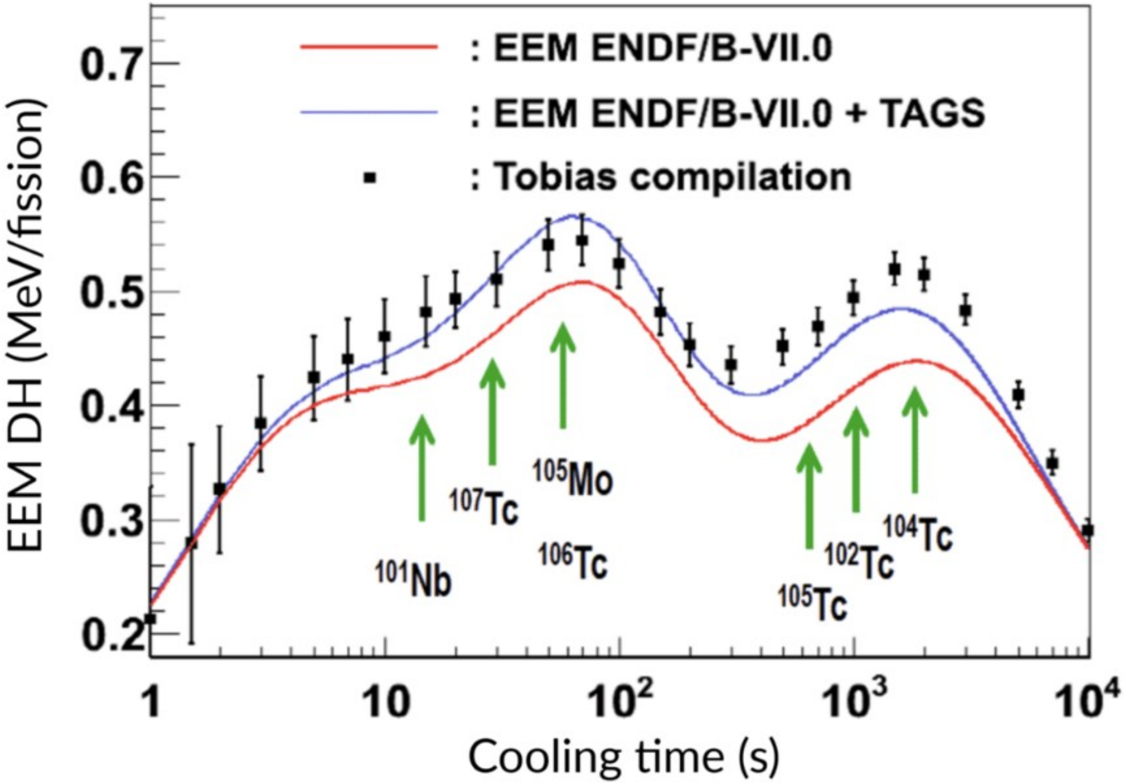
More details in: F. Esposito, *Fission yield uncertainty propagation with Monte Carlo method for decay heat calculation*, Master Thesis, 2025

Backup – Pandemonium effect

Efficiency of Ge detectors decreases as the energy of gamma ray increases → underestimation of mean gamma energy and overestimation of mean beta energy



M. Fleming and J.-C. Sublet. "*Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events*". June 2015. doi: 10.13140/RG. 2.1.1003.8168



A. Algora et al. "*Reactor Decay Heat in 239Pu: Solving the γ Discrepancy in the 4–3000-s Cooling Period*". In: Phys. Rev. Lett. 105 (20 Nov. 2010)