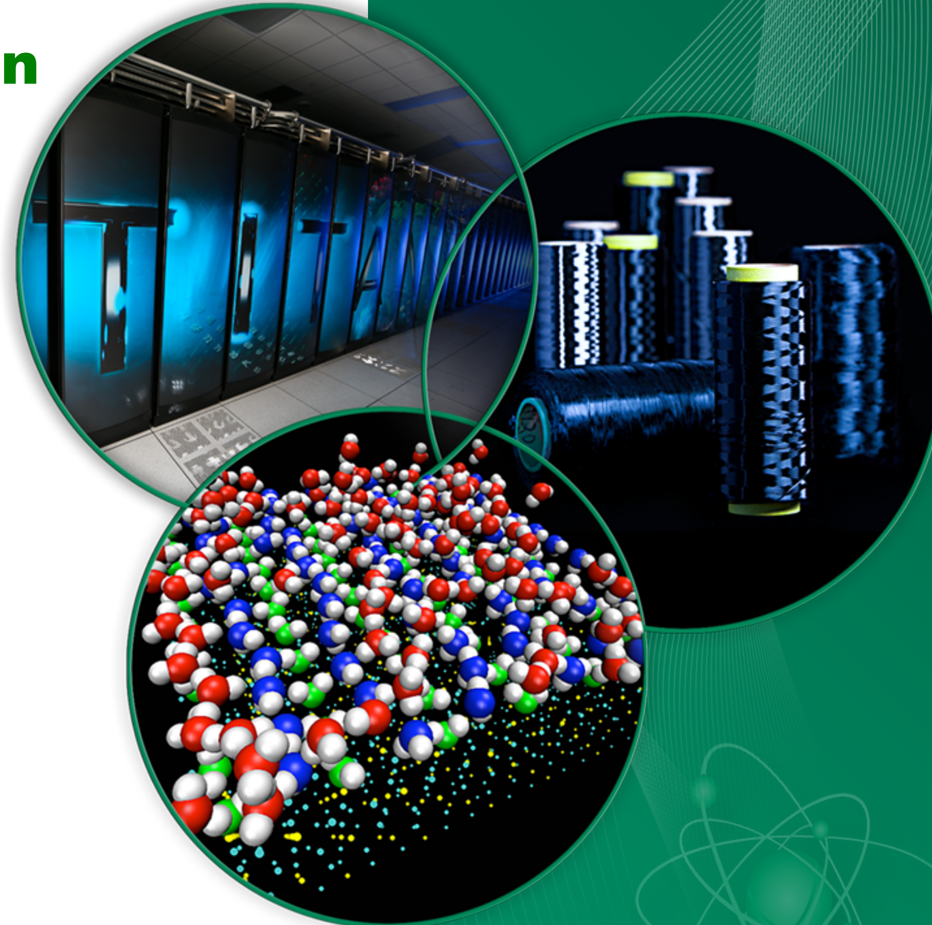
Applications of Decay Data and Fission Product Yield Covariance Matrices in Uncertainty Quantification on Decay Heat



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FPY covariance strategies

We developed several methodologies to generate covariance matrices on Independent Fission Product Yields (FPY) with no intent to re-evaluate the ENDF/B-VII.1 library

Methodology 1: Based on five Gaussian and Wahl models
- Sum/Mass yields correlations are included (five Gaussian model or, in the future, GEF code)
- Fractional yield correlations based on Wahl's model parameters

Methodology 2: Bayesian Method (T. Kawano)
- Useful to generate evaluations for independent FPY
- Model to define Chain Mass yields depends on branching ratios
- Correlation matrix is sparse

ORNL already has now the capability to propagate decay data and FPY uncertainties and correlations. Perturbation factors are used by SAMPLER to estimate uncertainties on specific applications, such as decay heat

Definitions and constraints

Independent fission yield from the fission of a nucleus with mass number A_T and atomic number Z_f :

$$y \equiv y(A,Z,I;\vec{x}) \quad \text{where} \quad \vec{x} \equiv \vec{x}(A_f, Z_f, E)$$

For neutron-induced fission, $A_f = A_T + 1$ (compound nucleus)
For spontaneous fission, $A_f = A_T$

Generally, for a semi-empirical model, the independent fission yield depends on a set of parameters:

$$\vec{x} = \{\vec{\mu}(A_f, Z_f, E), \vec{\lambda}(A_f, Z_f, E)\}$$

$$y = Y(A;\vec{\mu}) \times f(A,Z;\vec{\lambda}) \times R(A,Z,I)$$

Sum yield for a mass chain A
(chain yield C(A) can differ by a few percent)

Fractional independent yield

Isomeric yield ratio
(based on the Madland and England functions)

$\nu(E)$ Average number of nucleons emitted before and after fission

$if \quad E \leq 8 \quad MeV, \quad \nu(E) \approx \bar{\nu}_F(E)$ (prompt fission neutrons)

Constraints

$$\sum_Z f(A,Z;\lambda) = 1 \quad \forall\ A$$

$$\sum_I R(A,Z,I) = 1 \quad \forall\ A,Z$$

$$Y(A) = \sum_{Z,I} y(A,Z,I;\vec{x}) \quad \forall\ A$$

$$\sum_{AZI} y(A,Z,I;\vec{x}) = 2$$

(two fragments per fission)

$$\sum_{AZI} A y(A,Z,I;\vec{x}) = A_f - \nu(E)$$

$$\sum_{AZI} Z y(A,Z,I;\vec{x}) = Z_f$$

Model for Sum and Chain Yields

$$\psi_i^{\pm}(A) = (\sqrt{2\pi}\sigma_i)^{-1} e^{-(A-\bar{A}(\nu)\pm D_i)^2/2\sigma_i^2}$$

$$Y(A;\vec{\mu}) = \sum_{i=1}^{2} N_i(\psi_i^{+} + \psi_i^{-}) + N_3\psi_3$$

(Five Gaussian Model)

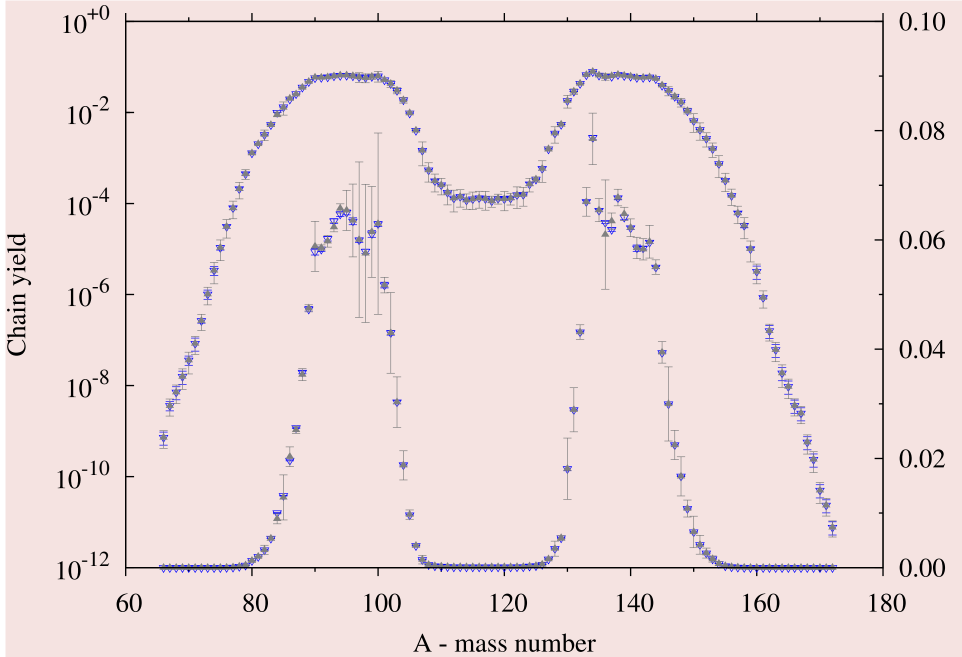
$$\psi_3(A) = (\sqrt{2\pi}\sigma_3)^{-1} e^{-(A-\bar{A}(\nu))^2/2\sigma_3^2}$$

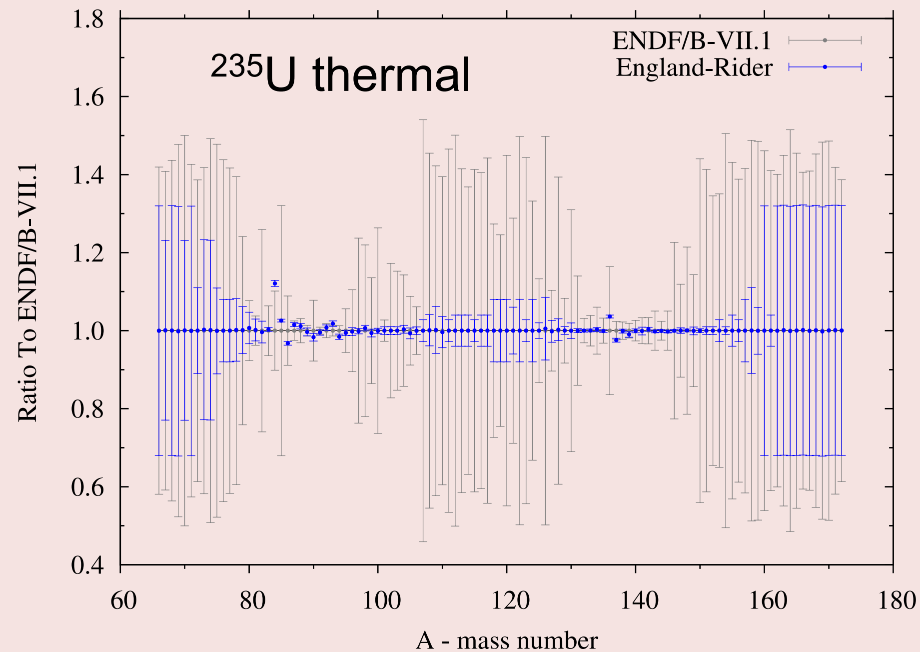
$$\vec{\mu} = \{\bar{A}(\nu), N_1, \sigma_1, D_1, N_2, \sigma_2, D_2, \sigma_3\}$$

Set of 8 model parameters

$$N_3 = 2(1 - N_1 - N_2) \quad \Rightarrow \sum_A Y(A;\vec{\mu}) = 2$$

For ^{235}U at neutron thermal energy chain (England-Rider) and sum yields (ENDF/B-VII. 1) differ by a few percent (see Figures). We approximate the sum yield with the 5 Gaussian Model.





Model for Independent Fractional Yield

$$f(A,Z;\vec{\lambda}) = \frac{1}{2} N(A) F(A;\vec{f}_r) \left(\sqrt{\frac{\pi}{2}} \sigma_z(A';\vec{s}_r) \right)^{-1} \int_{Z-1/2}^{Z+1/2} e^{-\frac{[Z'-Z_p(A';\vec{d}_r)]^2}{2\sigma_z(A';\vec{s}_r)}} dZ'$$

$$\vec{\lambda} = \{\vec{f}_r, \vec{s}_r, \vec{d}_r\}$$

$$A' = A + \nu_p$$

(Mass number corrected to account for post fission neutrons)

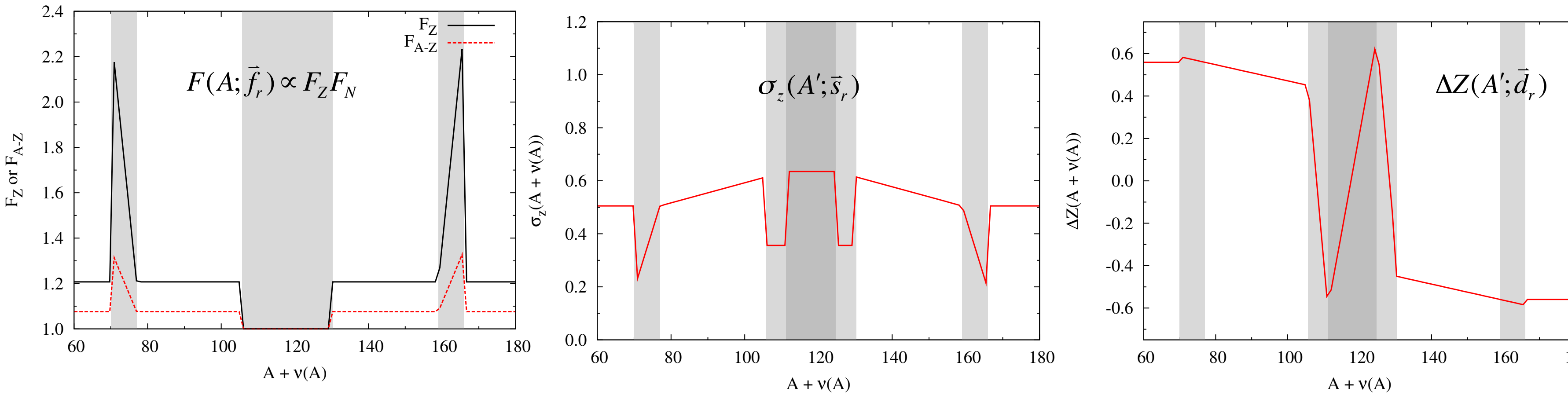
Normalization factor to guarantee unitary

Function for the even-odd effects in proton and neutron pairing

$$erf\left(\frac{Z - Z_p + 1/2}{\sigma_z \sqrt{2}}\right) - erf\left(\frac{Z - Z_p - 1/2}{\sigma_z \sqrt{2}}\right)$$

$$Z_p = (A + \nu_p) Z_f / A_f + \Delta Z(A + \nu_p; \vec{d}_r)$$

^{235}U thermal (Wahl model systematics)



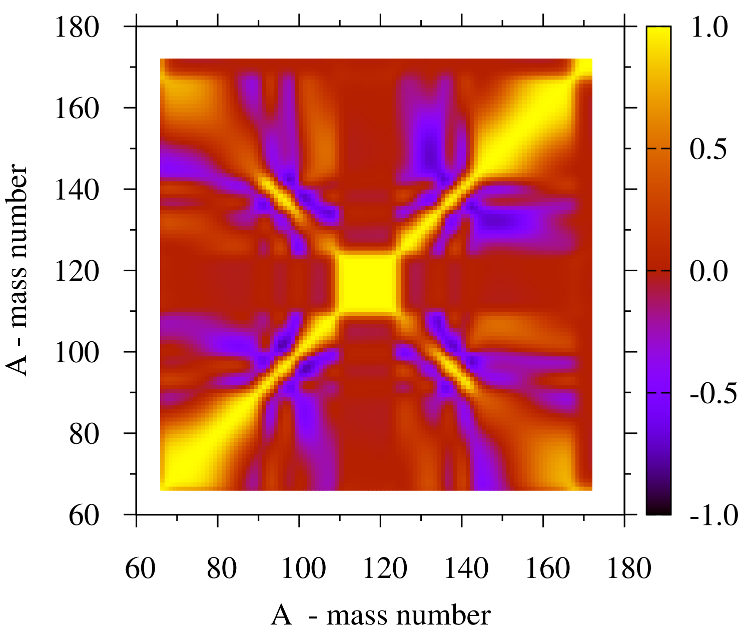
Covariance Matrix for Independent Yield

$$\langle \Delta y_c \Delta y_{c'} \rangle = \sum_{k,\ell} \frac{\partial y_c(\vec{x})}{\partial x_k} \langle \Delta x_k \Delta x_\ell \rangle \frac{\partial y_{c'}(\vec{x})}{\partial x_\ell} \qquad c(c') \equiv A, Z, I(A', Z', I')$$

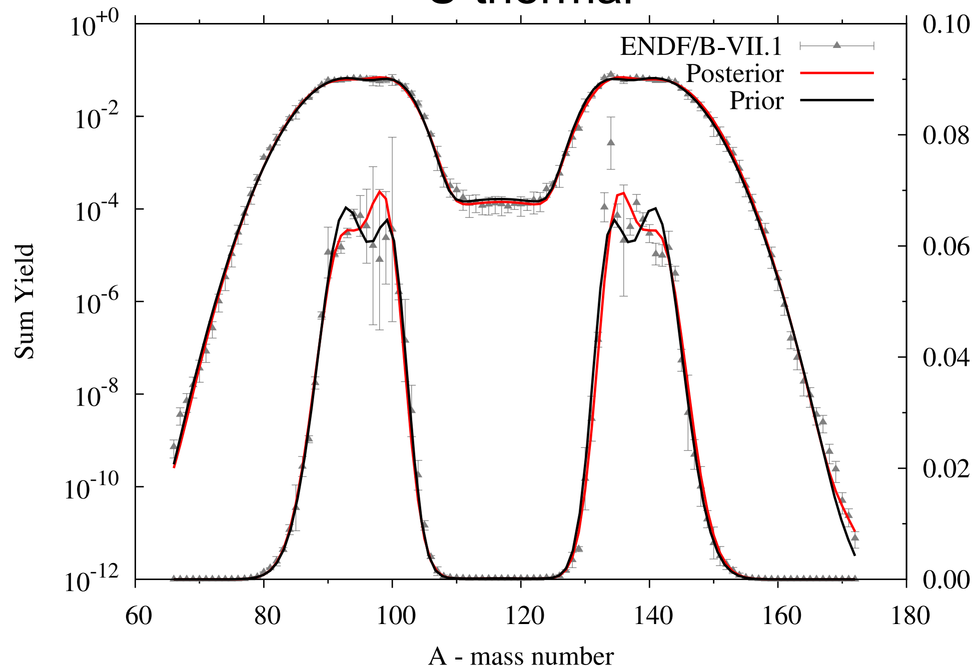
$$\langle \Delta x_k \Delta x_\ell \rangle \equiv \begin{pmatrix} \langle \Delta \mu_i \Delta \mu_{i'} \rangle & 0 \\ 0 & \langle \Delta \lambda_j \Delta \lambda_{j'} \rangle \end{pmatrix} \qquad \langle \Delta \lambda_j \Delta \lambda_{j'} \rangle \equiv \begin{pmatrix} \langle \Delta f_{r,a} \Delta f_{r,a'} \rangle & 0 & 0 \\ 0 & \langle \Delta s_{r,b} \Delta s_{r,b'} \rangle & 0 \\ 0 & 0 & \langle \Delta d_{r,c} \Delta d_{r,c'} \rangle \end{pmatrix}$$

Diagonal matrix: no correlations between model parameters
Uncertainties on model parameters taken form Wahl systematics

Non diagonal matrix: correlations derived from fitting ENDF/B-VII.1 sum yields



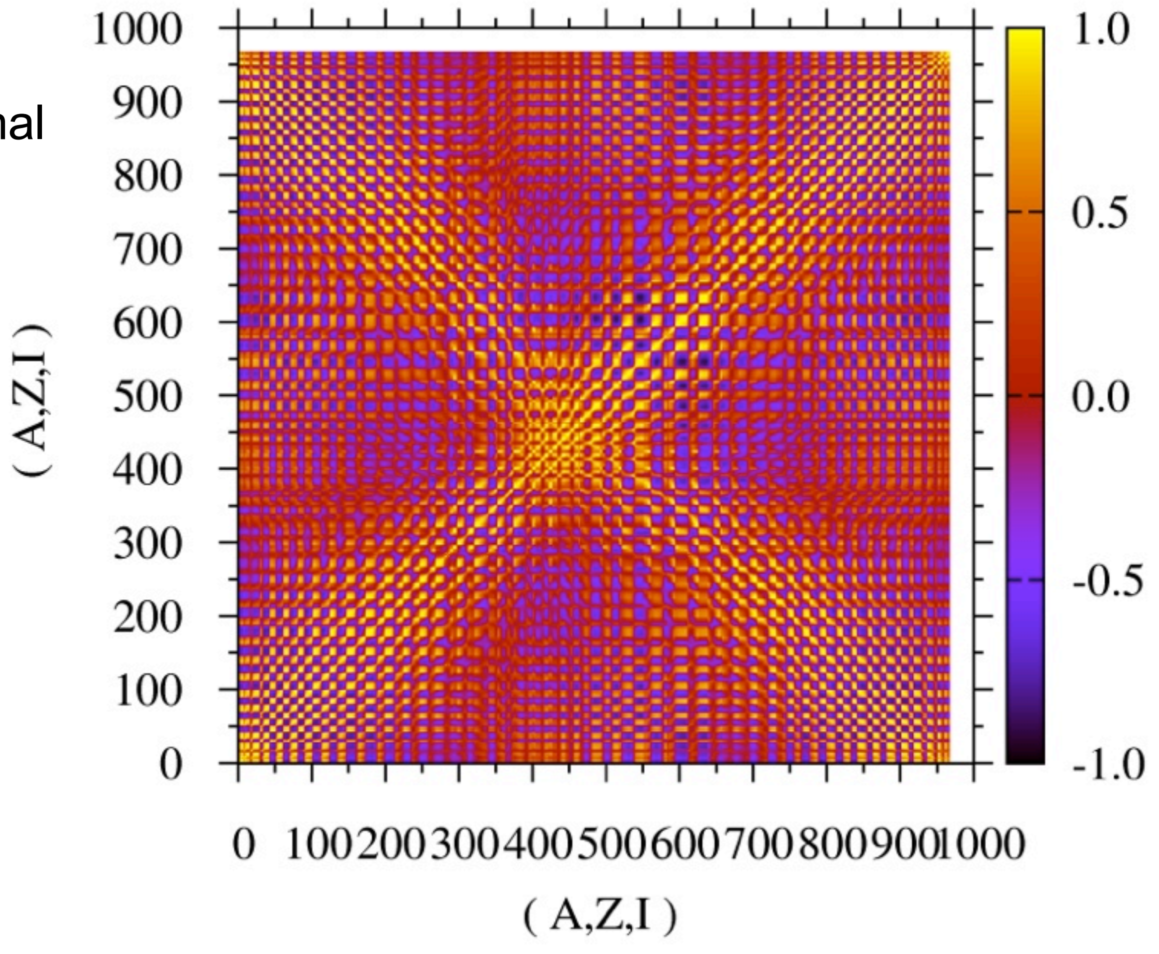
^{235}U thermal



Covariance Matrix for Independent Yield

The full covariance matrix is 1237X1237 elements (975x975 different from zero)
The matrix is arranged according to the list of nuclides in ENDF/B-VII.1 evaluation

^{235}U thermal



Bayesian Method (T. Kawano)

$$P_1 = P_0 - P_0 S^t (S P_0 S^t + Z)^{-1} S P_0$$

$$\vec{y}_1 = \vec{y}_0 + P_1 S^t Z^{-1} [\vec{Y} - F(\vec{y}_0)]$$

- The model is defined by the relations

$$Y_i = \sum_j c_j \delta(A_i = A_j) \delta(T_{1/2} >> T_\infty)$$

where

$$c_j^{k+1} = y_j + \sum_{j,\ell} c_\ell^k b_{j\ell} \quad and \quad F(\vec{y}) = \vec{Y}$$

$$P_2 = P_1 - P_1 T^t (T P_1 T^t + \sigma_T^2)^{-1} T P_1$$

$$\vec{y}_2 = \vec{y}_1 + P_2 T^t \sigma_T^{-2} [2 - T^t \vec{y}_1]$$

$$T^t I = 2$$

Constraint I : total yield sums to 2

$$P_3 = P_2 - P_2 U^t (U P_2 U^t + \sigma_U^2)^{-1} U P_2$$

$$\vec{y}_3 = \vec{y}_2 + P_3 U^t \sigma_U^{-2} [A_f - \nu - U^t \vec{y}_2]$$

$$U^t I = A_f - \nu$$

Constraint II on the mass number

$$P_4 = P_3 - P_3 V^t (V P_3 V^t + \sigma_V^2)^{-1} V P_3$$

$$\vec{y}_4 = \vec{y}_3 + P_4 V^t \sigma_U^{-2} [Z_f - V^t \vec{y}_3]$$

$$V^t I = Z_f$$

Constraint III on the charge number

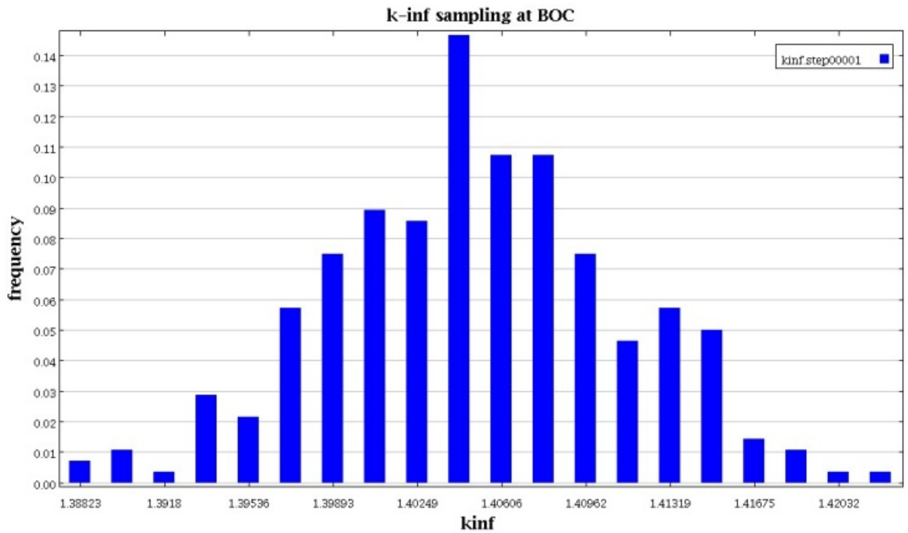
Implementation of Uncertainty Analysis (Havluj and Williams)

SAMPLER: An automated stochastic nuclear data sampling approach is implemented in the next release of SCALE (6.2 beta 1)

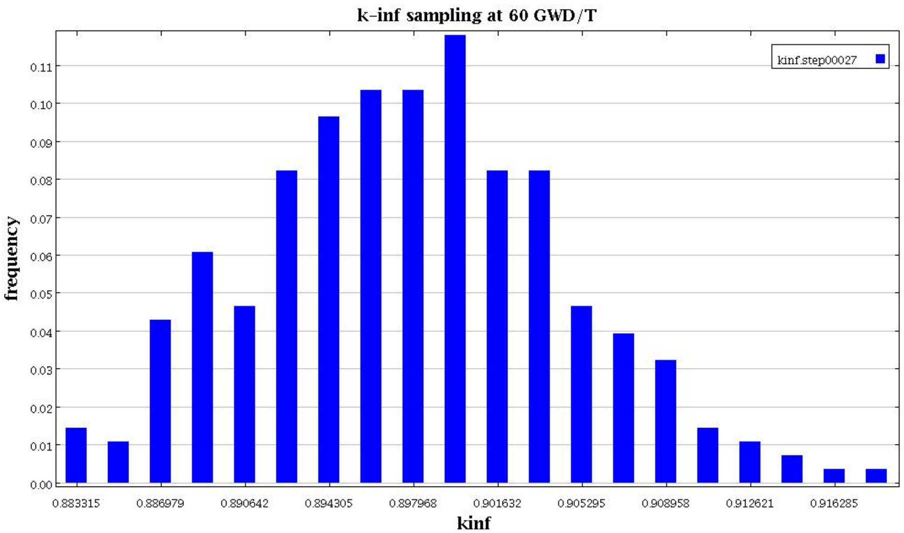
- **Defines uncertainty distributions and correlations for all nuclear data**
  - **Reaction cross sections**
  - **Fission Product Yields**
  - **Nuclear decay data**
- **Executes any SCALE code using perturbed nuclear data and design parameters for uncertainty analysis**
- **Performs parallel computations using MPI or OpenMP**
- **Response uncertainty computed by automated statistical analysis of output response distribution**

Sampled Frequency Distributions

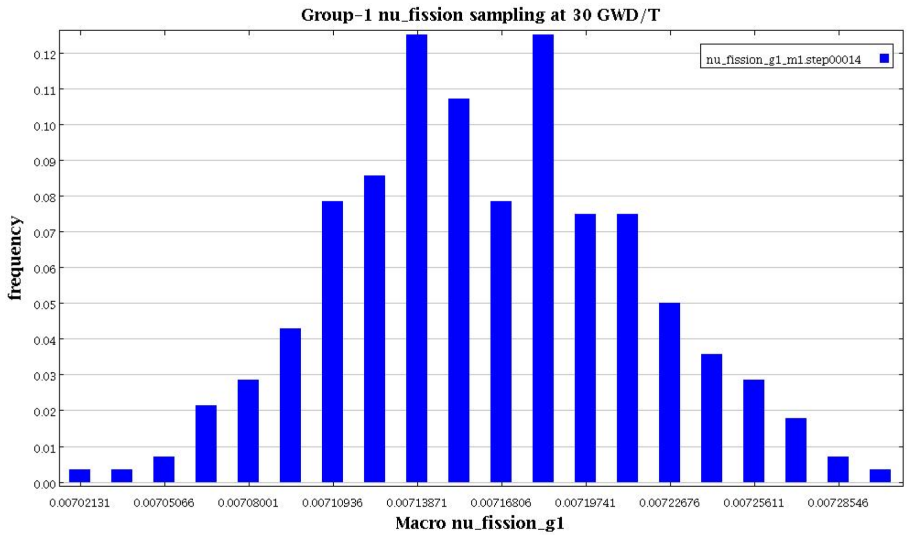
K_{inf} ; 0 GWD/T



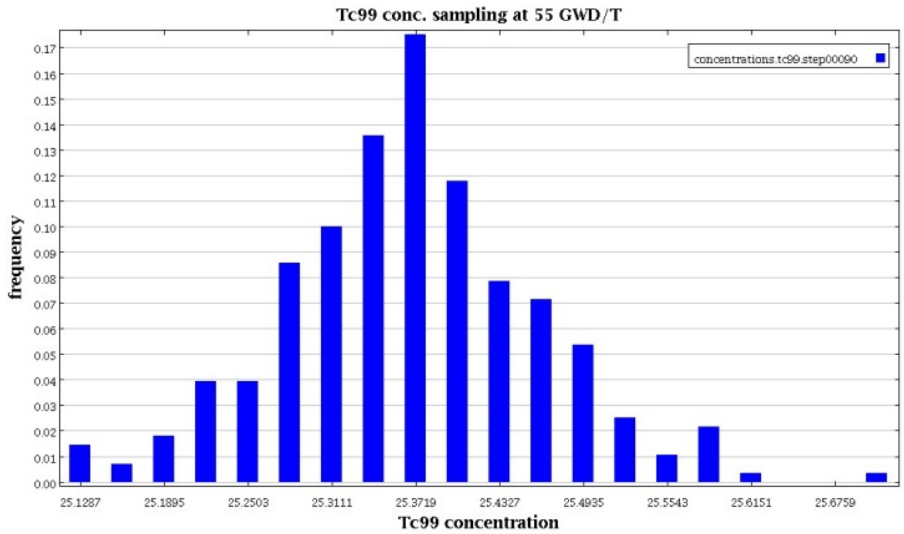
K_{inf} ; 60 GWD/T



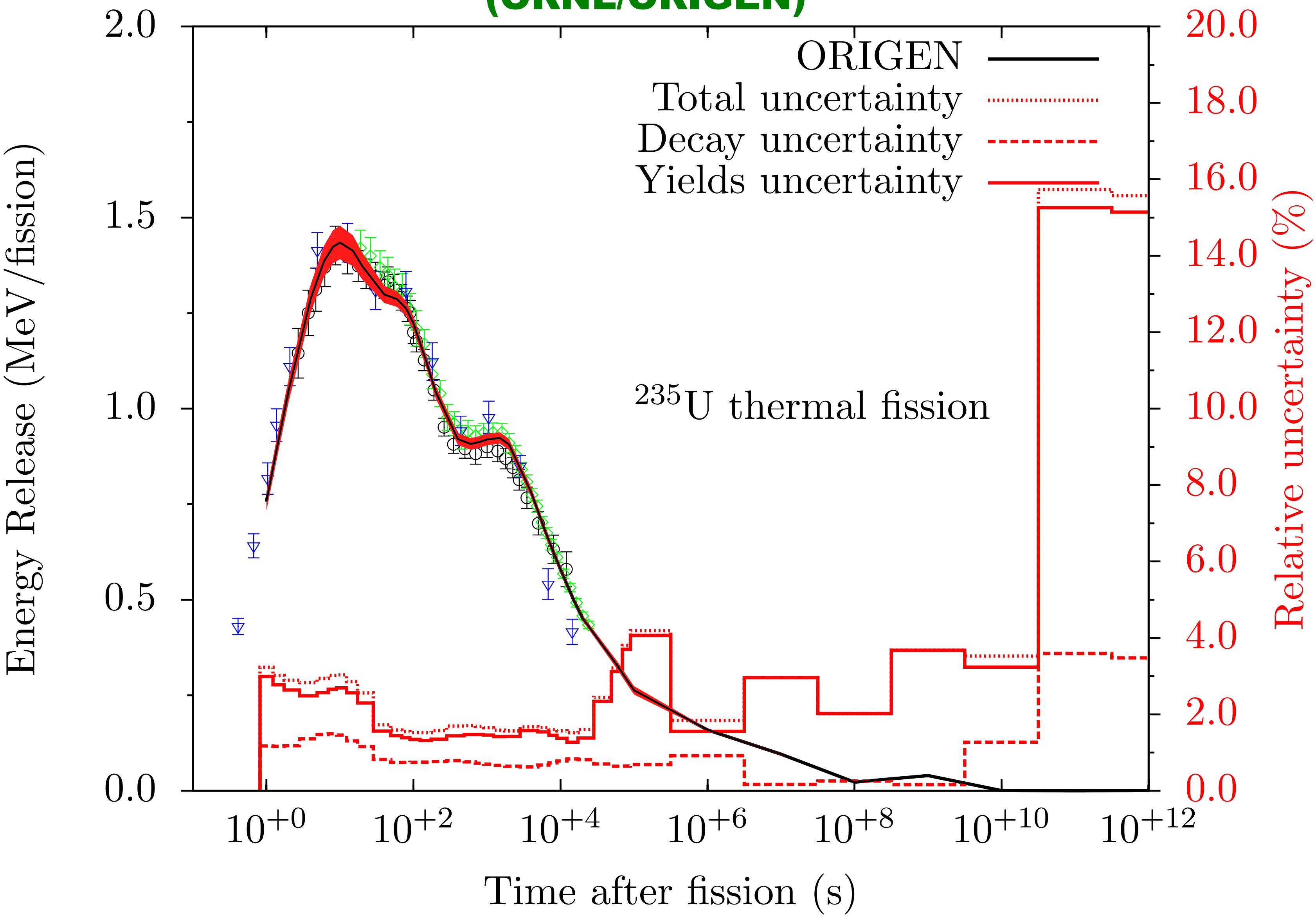
Group 1 nu-fission ; 30 GWD/T



Tc-99 concentration; 50 GWD/T



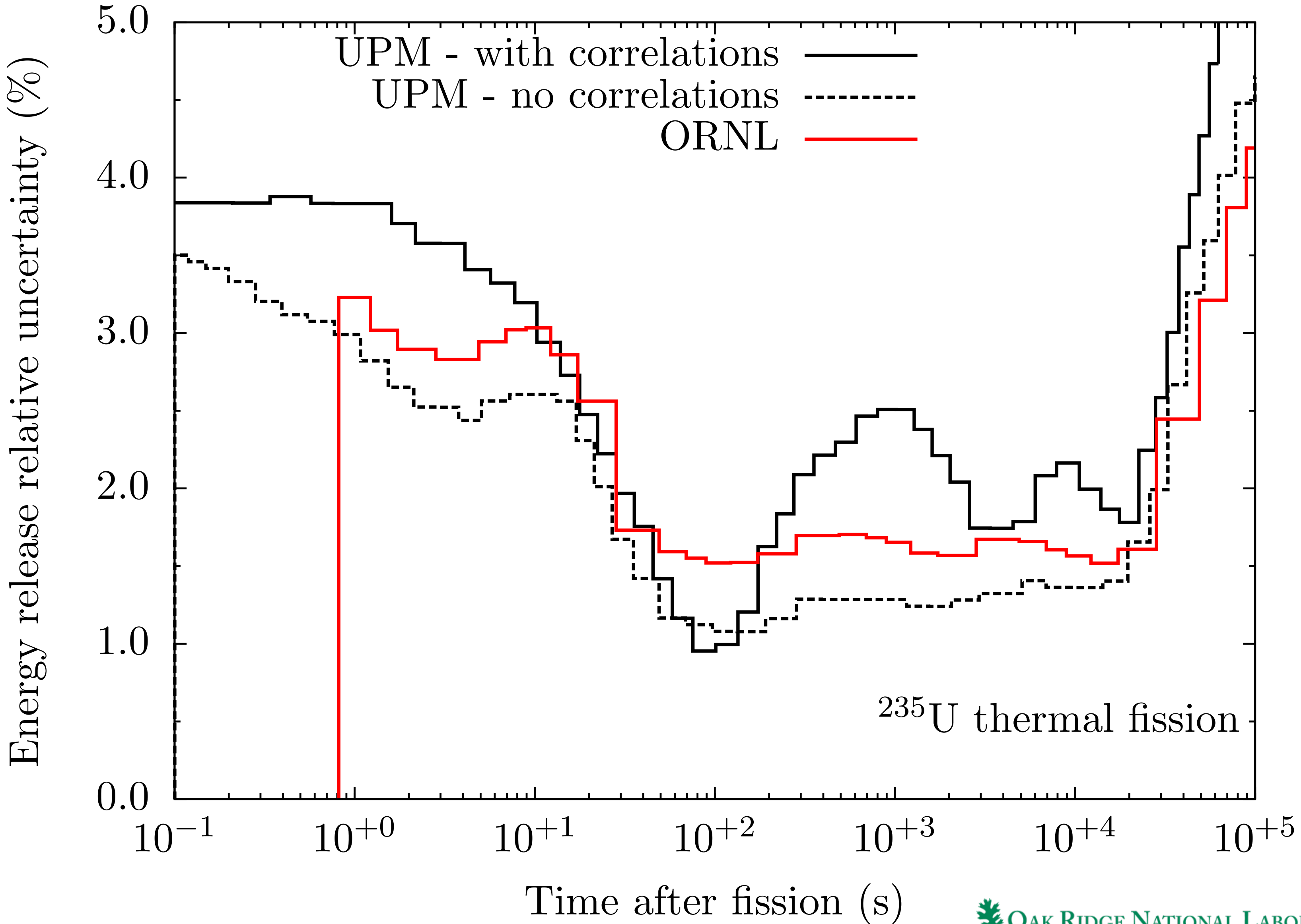
Uncertainty Estimate on Energy Release
(ORNL/ORIGEN)



Decay data uncertainties taken from ENDF/B-VII.1.

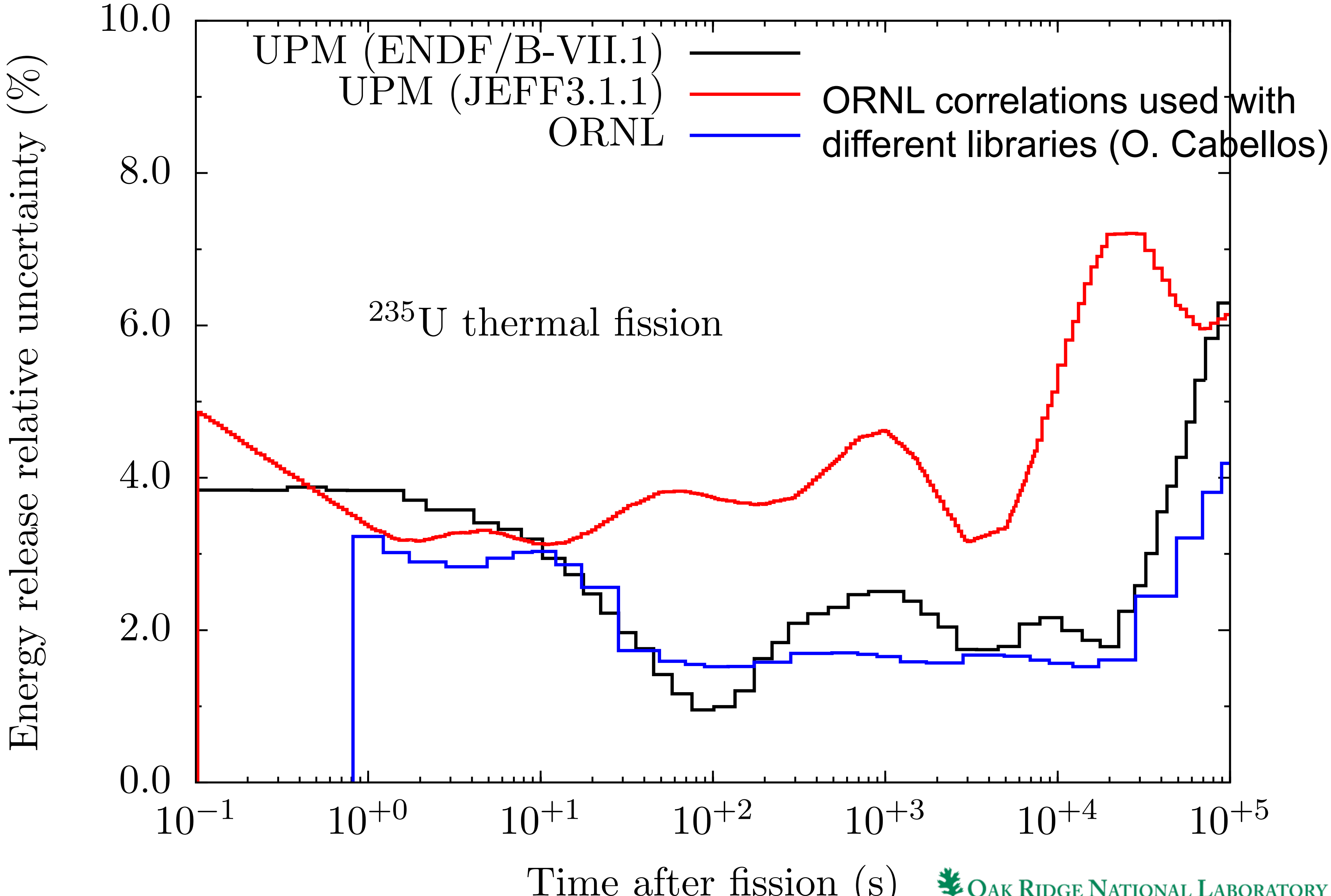
Uncertainty Estimate on Energy Release

ORNL vs Cabellos UPM (using ORNL correlation matrix)

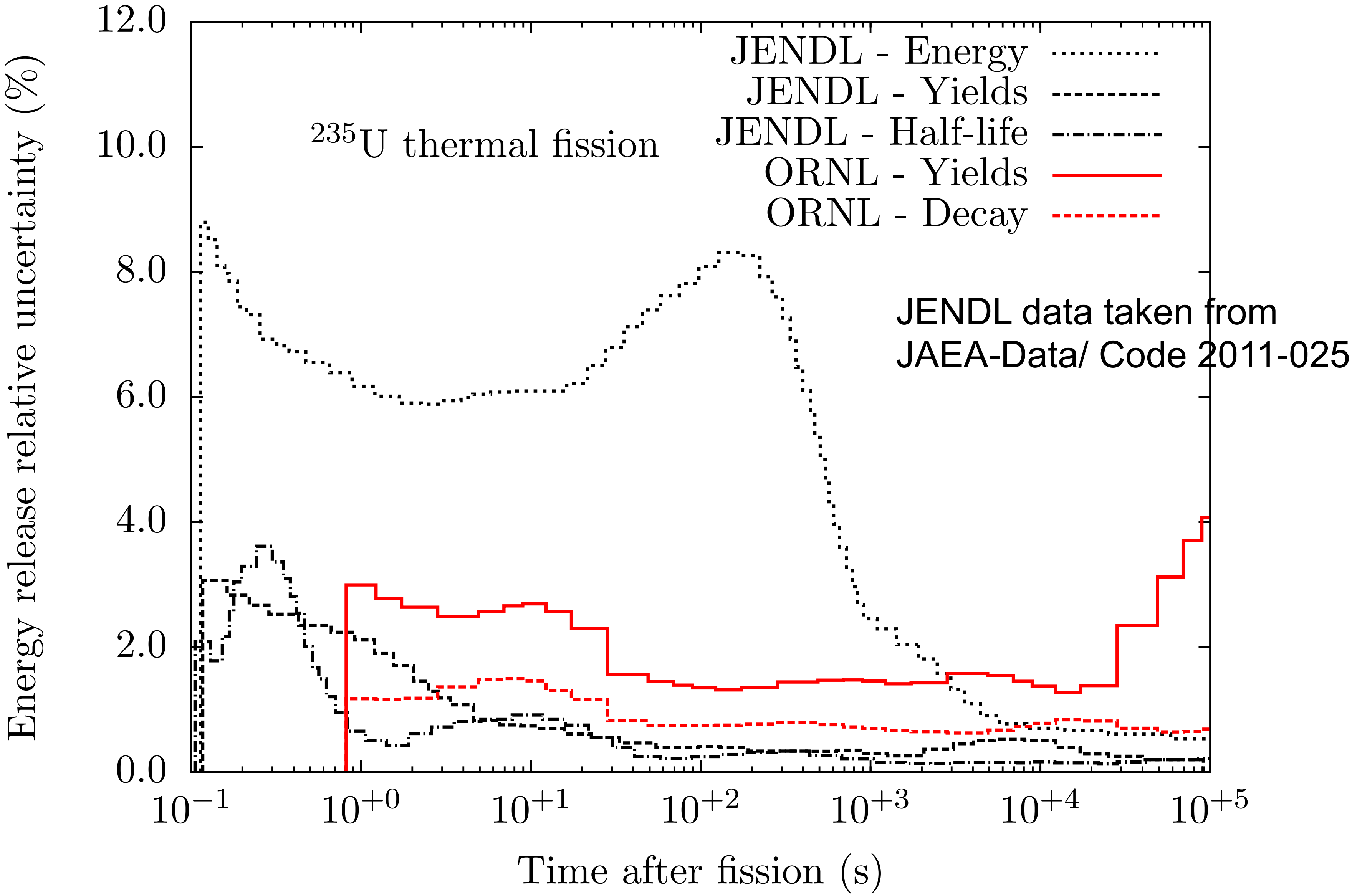


Uncertainty Estimate on Energy Release

ORNL vs Cabellos UPM (using ORNL correlation matrix)



Uncertainty Estimate on Energy Release
(ORNL vs Katakura JENDL)



SUMMARY / CONCLUSIONS

- We developed methodologies to generate covariance matrices on FPY

- We developed the capability to define uncertainty distributions for fission product yields, nuclear decay data

- We have preliminary results on the estimated uncertainty for Decay Heat (DH) calculations for the specific case of ^{235}U at thermal energy

- We tested our correlation matrix using different implementations (O. Cabellos)
    - The obtained relative uncertainties are overall in agreements
    - The correlations increase on average the relative uncertainties on DH

- We compared our results and those ones in JAEA-Data/Code2011-025 report. The relative uncertainties are driven by the total energy and not by fission product yield uncertainties

- Next step is to extend the analysis on decay heat calculations for other cases such as $^{239,241}Pu$ and ^{238}U