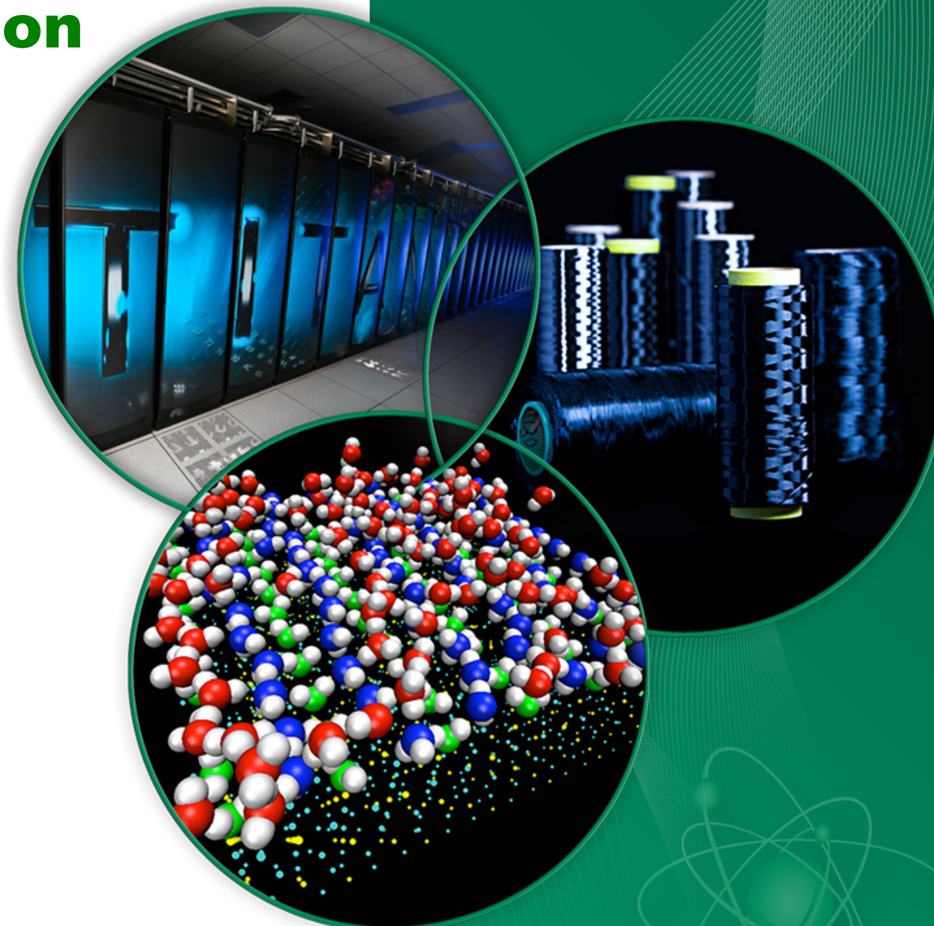
Consistent FPY Covariance Matrices in Uncertainty Quantification Analyses



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Outline

- **Methodologies to generate FPY covariance matrices**
- **Brief description of the Wahl's model (adopted methodology)**
- **Implementation in SAMPLER (Williams et al.)**
- **Results and uncertainty estimates on Decay heat and comparison with different implementations (Cabellos et al.)**
- **Issues found in ENDF/B-VII.1 FPY uncertainties for isotopic compositions (specific case on mass A=148)**
- **Possible solutions (Bayesian retroactive method)**
- **Conclusions and future work (complete set of FPY covariance matrices, format, etc.)**

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. Each methodology has some weak point.

Methodology 1: Based on five Gaussian and Wahl models

- Sum/Mass yields correlations are included (five Gaussian model)
- Fractional yield correlations based on Wahl's model parameters
- Estimation of parameter uncertainties to be updated

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

Methodology 3: GEF code (K.-H. Schmidt)

- Useful to generate chain mass and independent FPY covariance matrices
- Model (to define independent FPY and mass chain) is phenomenological
- Estimates on FPY uncertainty are, on average, comparable to ENDF/B-VII.0

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 and isotopic concentrations

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:

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

$$y = \underbrace{Y(A;\vec{\mu})}_{\text{Sum yield for a mass chain } A \text{ (chain yield C(A) can differ by a few percent)}} \times \underbrace{f(A,Z;\vec{\lambda})}_{\text{Fractional independent yield}} \times \underbrace{R(A,Z,I)}_{\text{Isomeric yield ratio (based on the Madland and England functions)}}$$

$\nu(E)$ 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)

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

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

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)

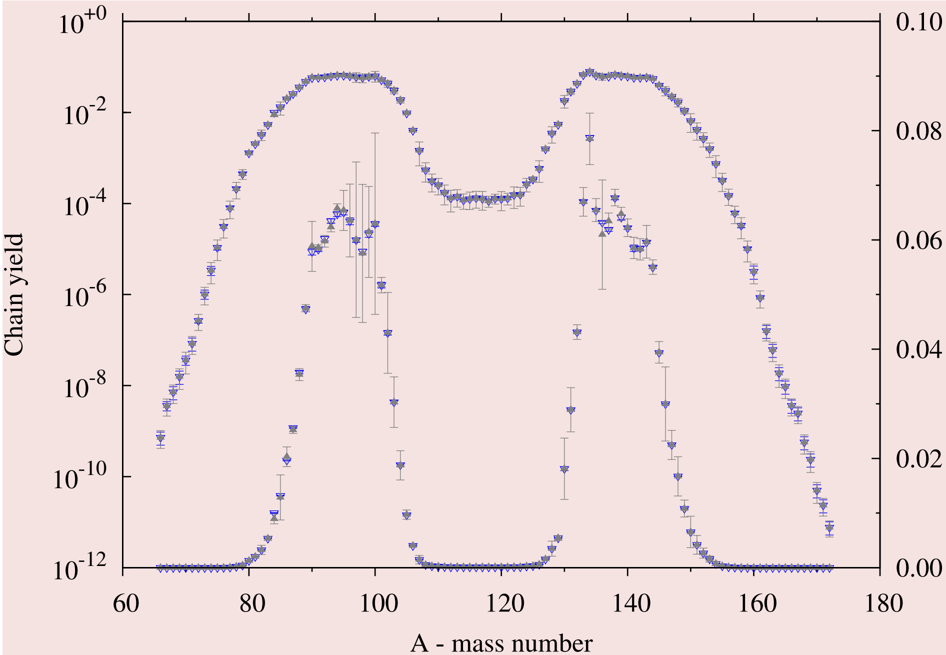
$$\psi_3(A) = (\sqrt{2\pi}\sigma_3)^{-1} e^{-(A-\bar{A}(\nu))^2/2\sigma_3^2}$$

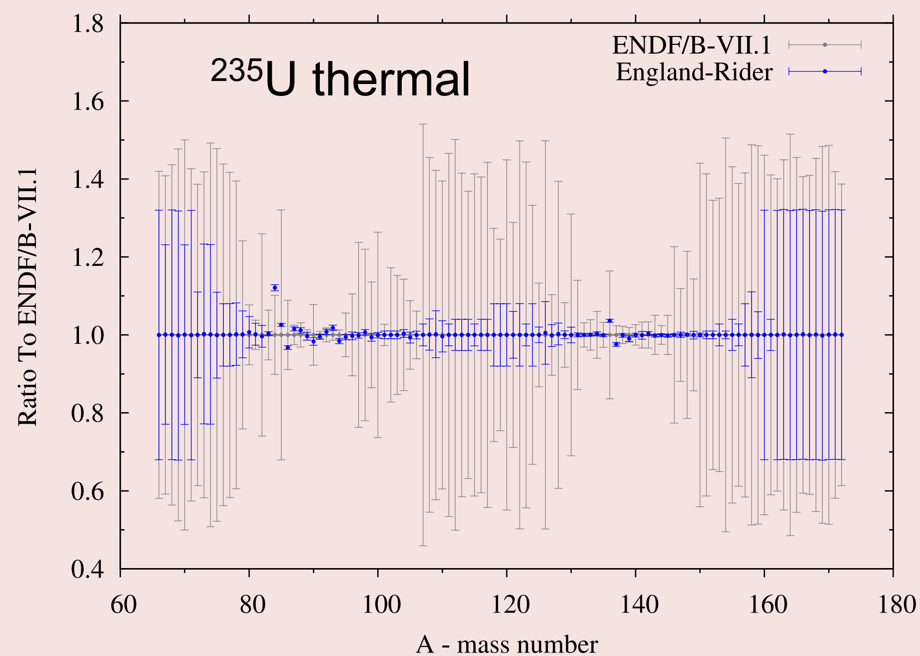
$$\vec{\mu} = \{\bar{A}(\nu), N_1, \sigma_1, D_1, N_2, \sigma_2, D_2, \sigma_3\}$$

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)

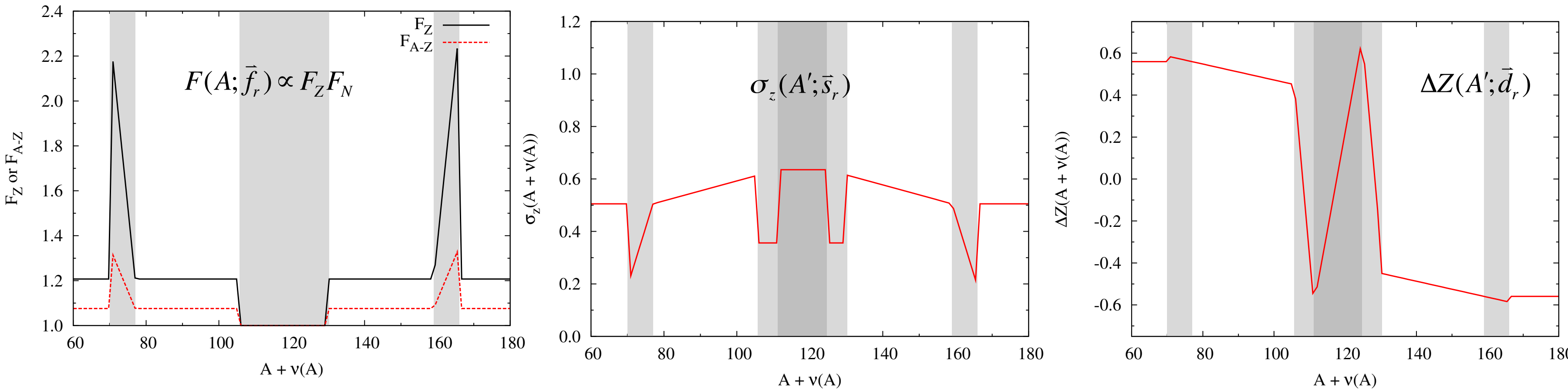
Normalization factor to guarantee unitary

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)



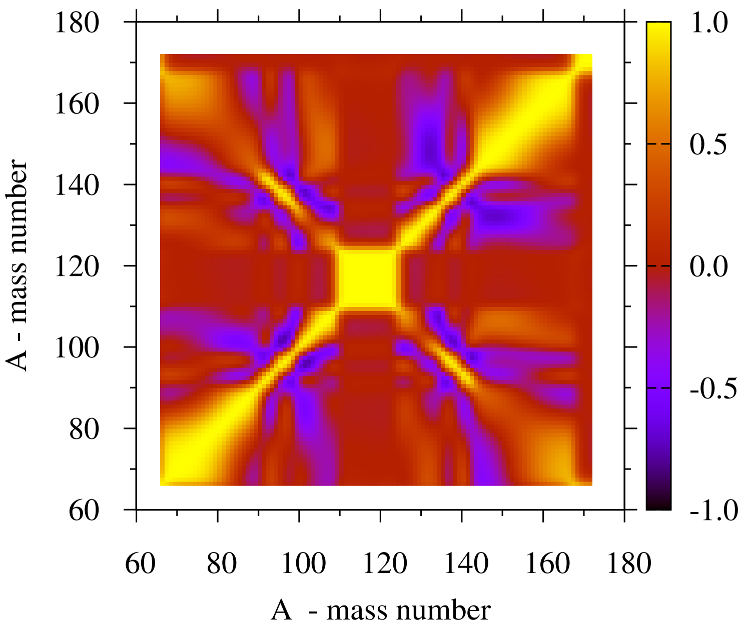
Covariance Matrix for Independent Yield

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

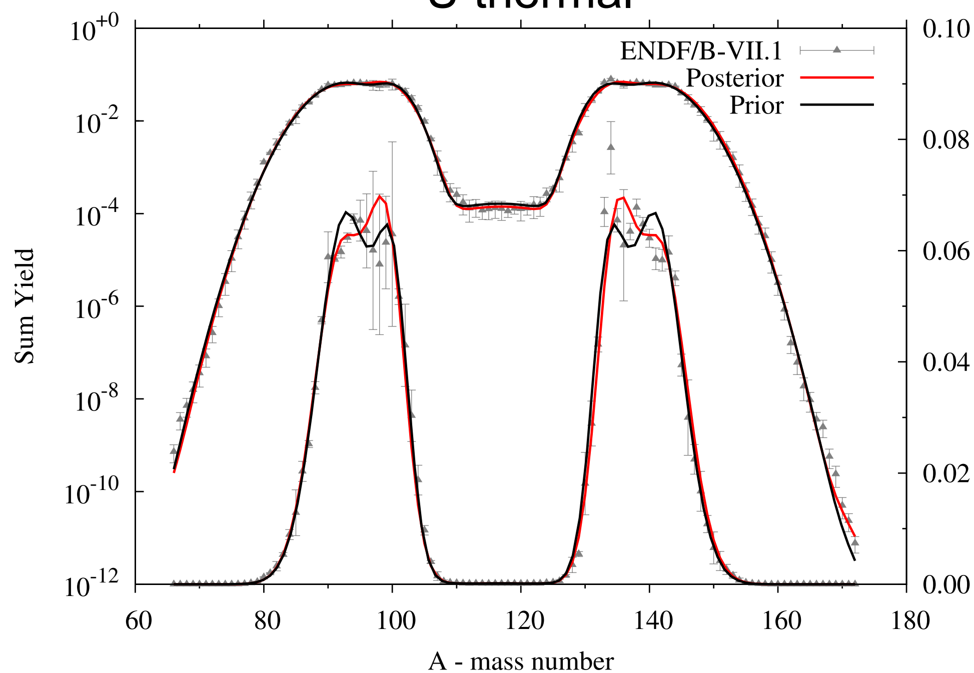
$$\left\langle \Delta x_k \Delta x_\ell \right\rangle \equiv \begin{pmatrix} \left\langle \Delta\mu_i \Delta\mu_{i'} \right\rangle & 0 \\ 0 & \left\langle \Delta\lambda_j \Delta\lambda_{j'} \right\rangle \end{pmatrix} \qquad \left\langle \Delta\lambda_j \Delta\lambda_{j'} \right\rangle \equiv \begin{pmatrix}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

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



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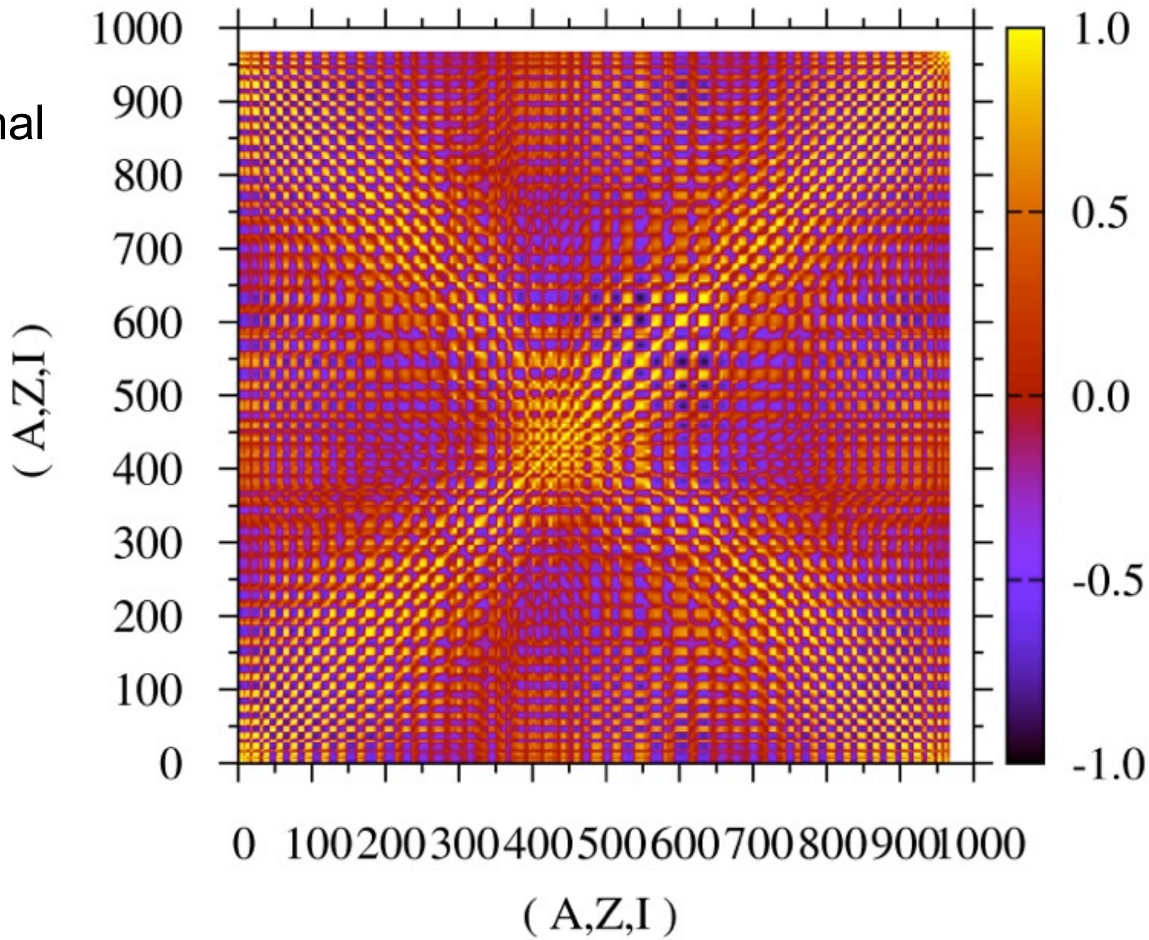
Covariance Matrix for Independent Yield

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

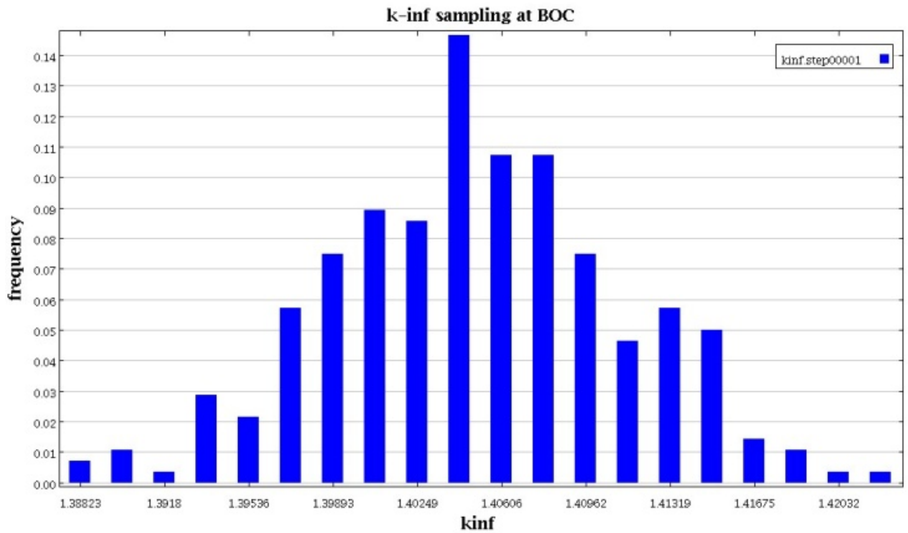
Implementation of Uncertainty Analysis (Williams et al.)

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

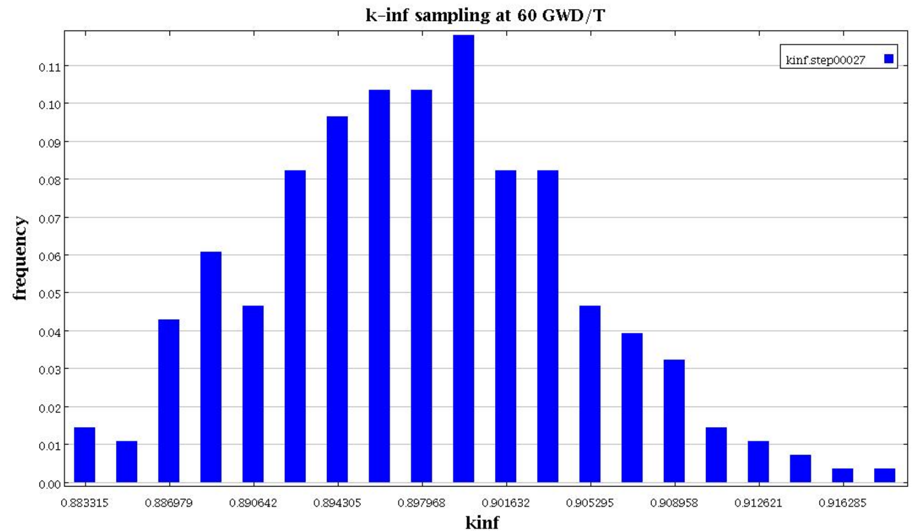
- Defines uncertainty distributions and correlations for all nuclear data
  - Reaction cross sections
  - Fission Product Yields
  - Nuclear decay data
- Executes any SCALE code using perturbed nuclear data and design parameters for uncertainty analysis
- Performs parallel computations using MPI or OpenMP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

Sampled Frequency Distributions

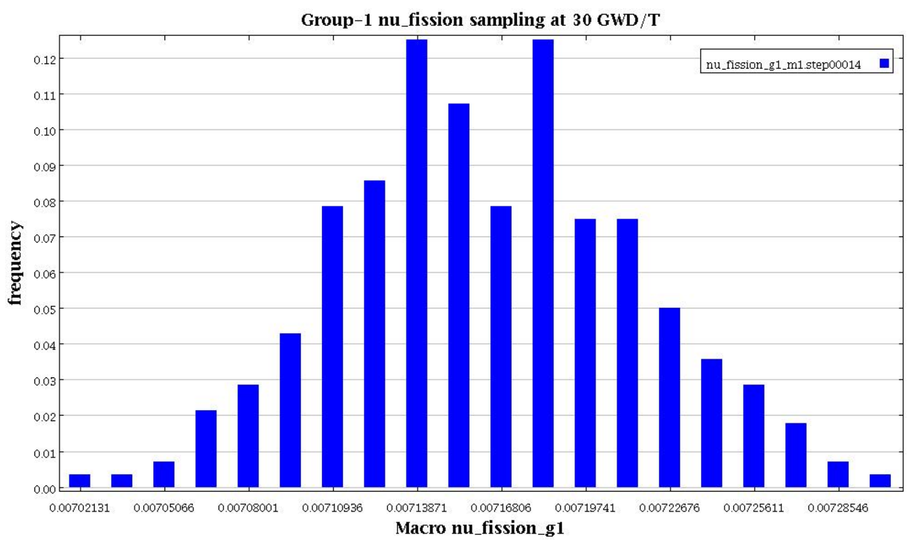
K_{inf} ; 0 GWD/T



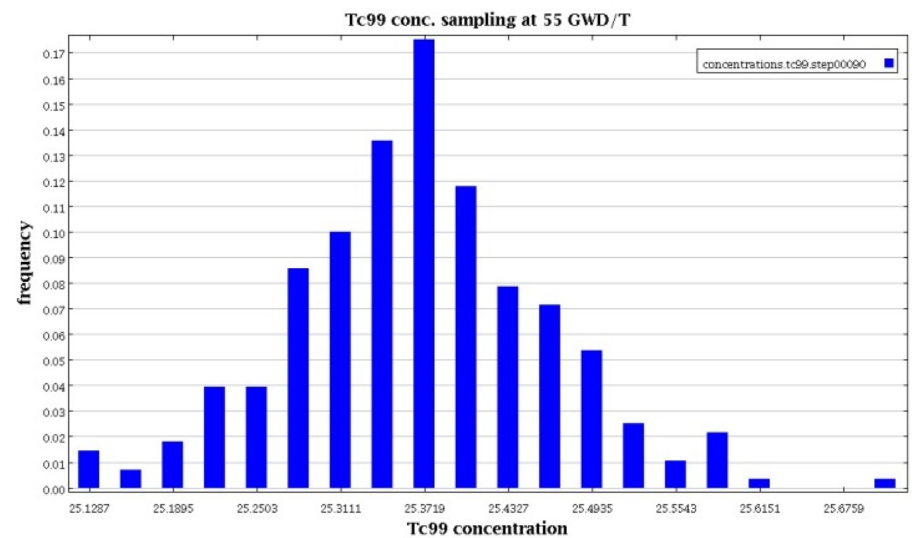
K_{inf} ; 60 GWD/T



Group 1 nu-fission ; 30 GWD/T

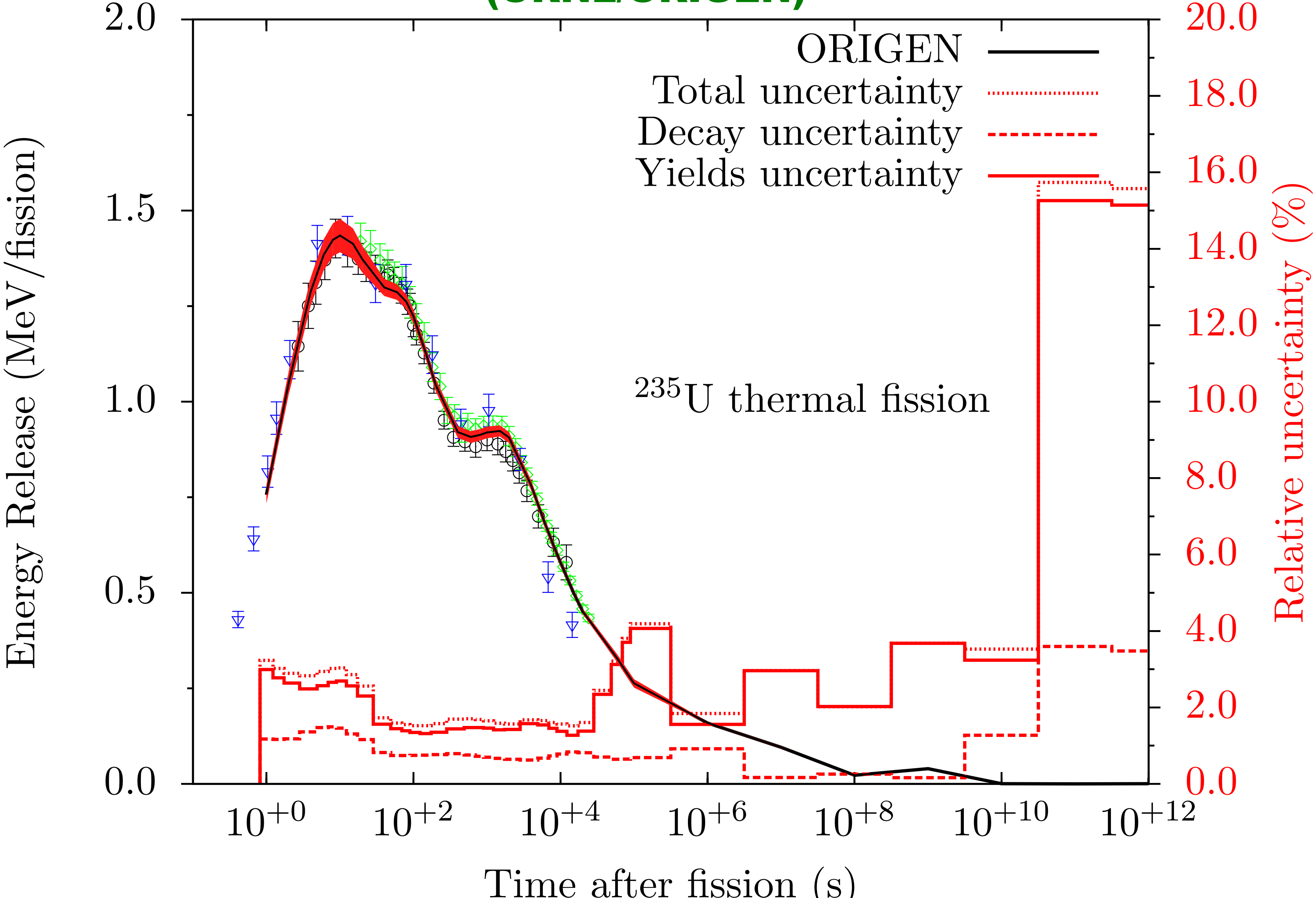


Tc-99 concentration; 50 GWD/T



Uncertainty Estimate on Energy Release

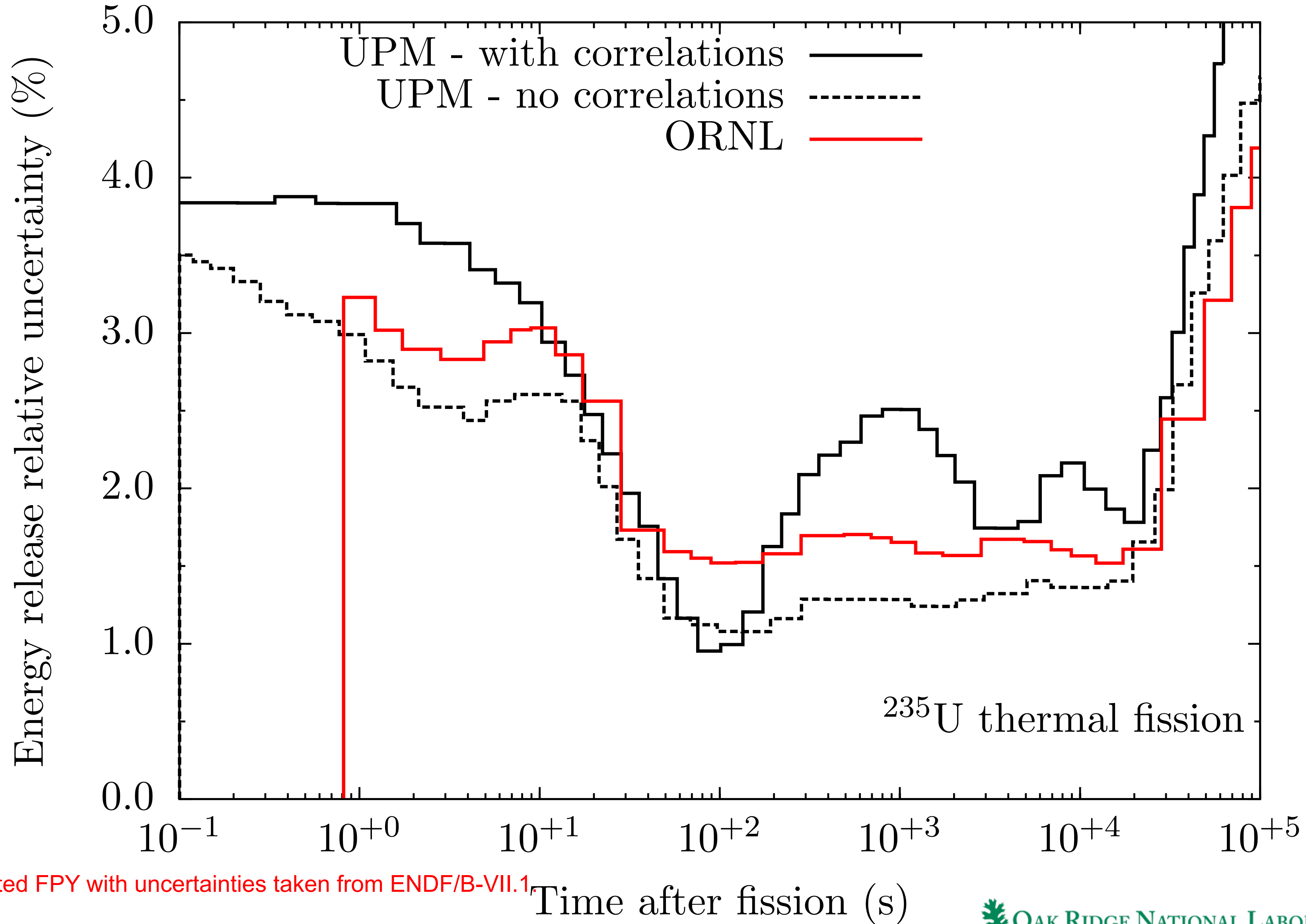
(ORNL/ORIGEN)



FPY and decay data uncertainties taken from ENDF/B-VII.1 (with correlations on FPY only)
No estimates on decay energy with no data uncertainties.

Uncertainty Estimate on Energy Release

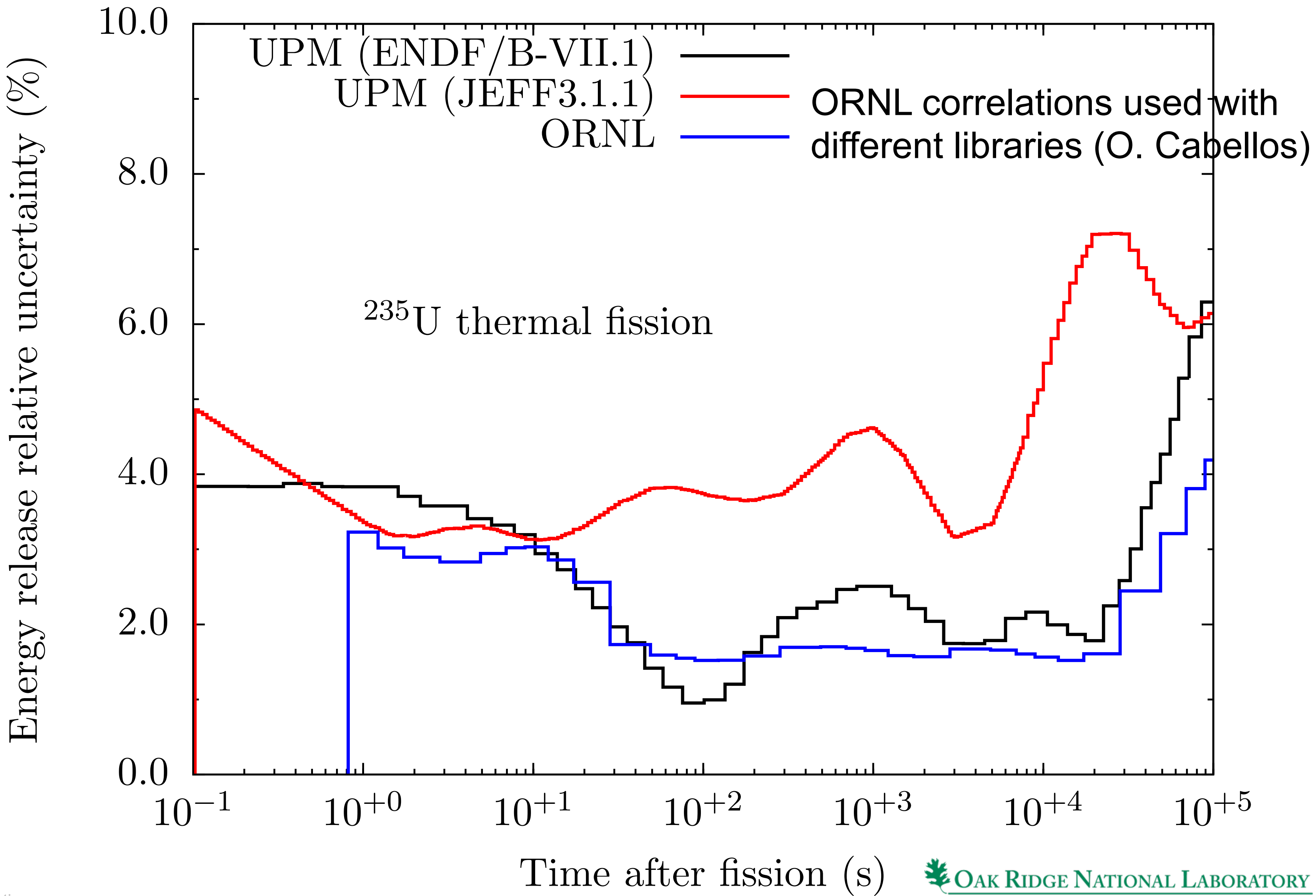
ORNL vs Cabellos UPM (using ORNL correlation matrix)



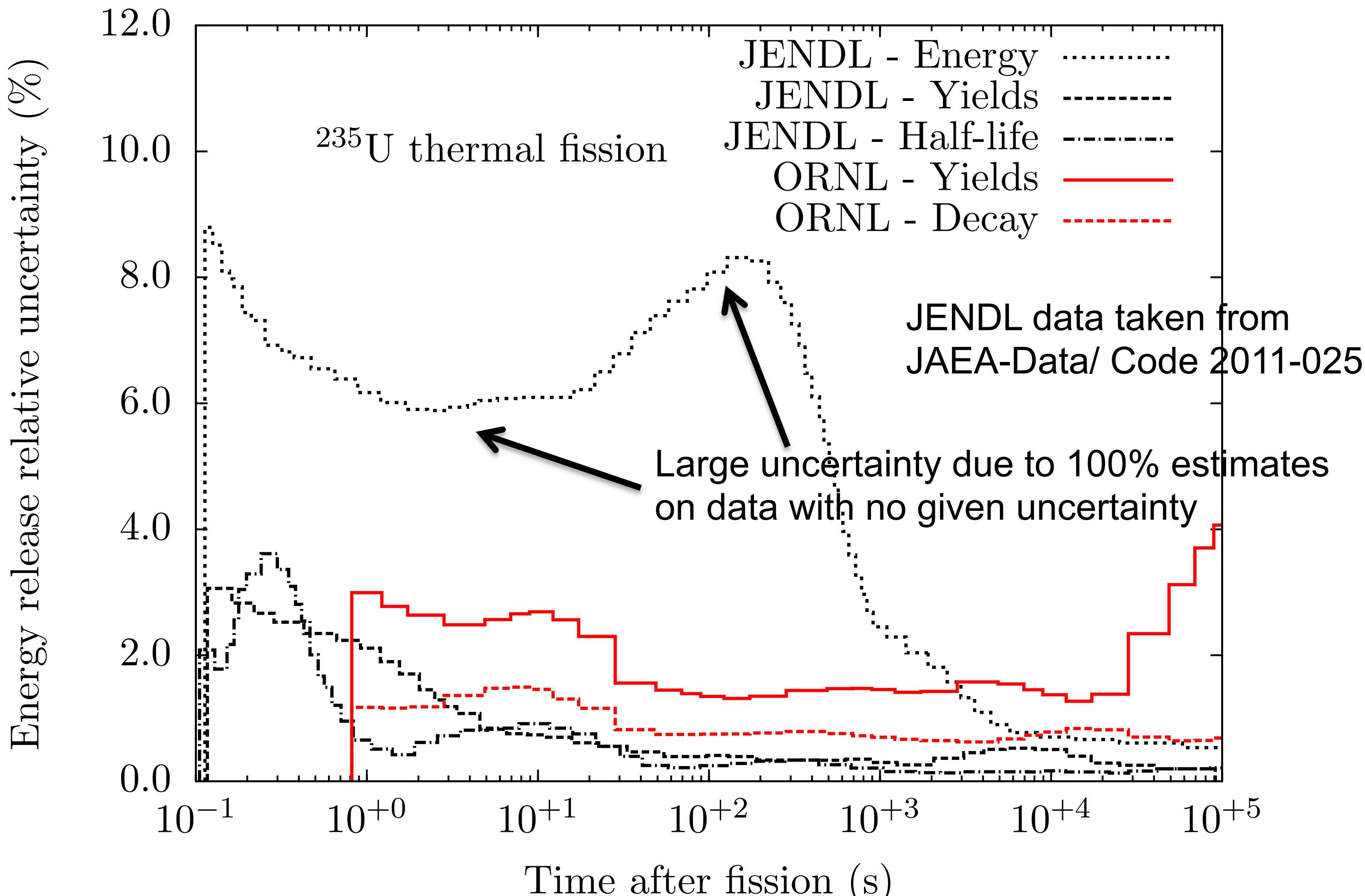
Correlated FPY with uncertainties taken from ENDF/B-VII.1

Uncertainty Estimate on Energy Release

ORNL vs Cabellos UPM (using ORNL correlation matrix)



Uncertainty Estimate on Energy Release
(ORNL vs Katakura JENDL)



FPY uncertainties taken from ENDF/B-VII.1.

Summary on Energy Release Results
(previous four plots)

- Energy release uncertainties were derived from
  - FPY uncertainties taken from ENDF/B-VII.1 plus correlations generated independently from the original evaluation procedure (plot 1). The effect of the correlations is to increase, on average, the uncertainties (plot 2).
  - Decay data uncertainties were taken from ENDF/B-VII.1 library. No estimates for decay energies given with no data uncertainties. The assumption of 100% uncertainty (e.g. JENDL on plot 4) for isotopes with no data uncertainty can lead to large differences.
- Test of ORNL covariance/correlation matrix on different implementations (Cabellos) was successful and showed comparable results (plot 3). Differences could derive from different decay schemes and uncertainties of the nuclear data library.

Issues with ENDF/B-VII.1 FPY uncertainties ("Rough" estimation of uncertainties)

- FPY evaluations in ENDF/B-VII.1 (except for ^{239}Pu) were adopted from England and Rider compilations in the 1990s
- FPY uncertainty estimates in ENDF/B-VII.1 were assigned and based on the absolute value of FPY data (64%, 32%, 16% uncertainty, etc.)
- Issues are found if ENDF/B-VII.1 uncertainties are propagated to compute uncertainty estimates on isotopic concentrations (e.g. chain A =148)
  - Uncertainties too large and inconsistent with cumulative yields
  - Lack of correlations
- Problems can be solved in different ways
  - Retroactive method which uses uncertainty information of cumulative yields (similar to Q matrices defined by Mills et al.)
  - New FPY evaluations with covariance matrices

Non–iterative Bayesian Method (NiB)

The non-iterative Bayesian update on a prior covariance matrix accounts for additional uncertainty information derived from the *cumulative* fission product yields. If M_0 is the prior covariance matrix, the updated matrix is defined as

$$M = (M_0^{-1} + SV^{-1}S^T)^{-1}$$

where *V* is the covariance matrix of the cumulative product yields and *S* (S^T) is the sensitivity (transpose) with matrix elements defined as

$$S_{lk} = \frac{\partial c_l(\vec{I};b)}{\partial I_k}$$

Where *c* are the cumulative yields for a specific chain with mass number *A* defined by the set of independent yields *I* belonging to the same chain. The function that relates the cumulative to the independent yields depends on a set of branching ratios *b* as

$$c(\vec{I};b) = \sum_i \prod_j b_{ij} I_j$$

Example on A=148 mass chain

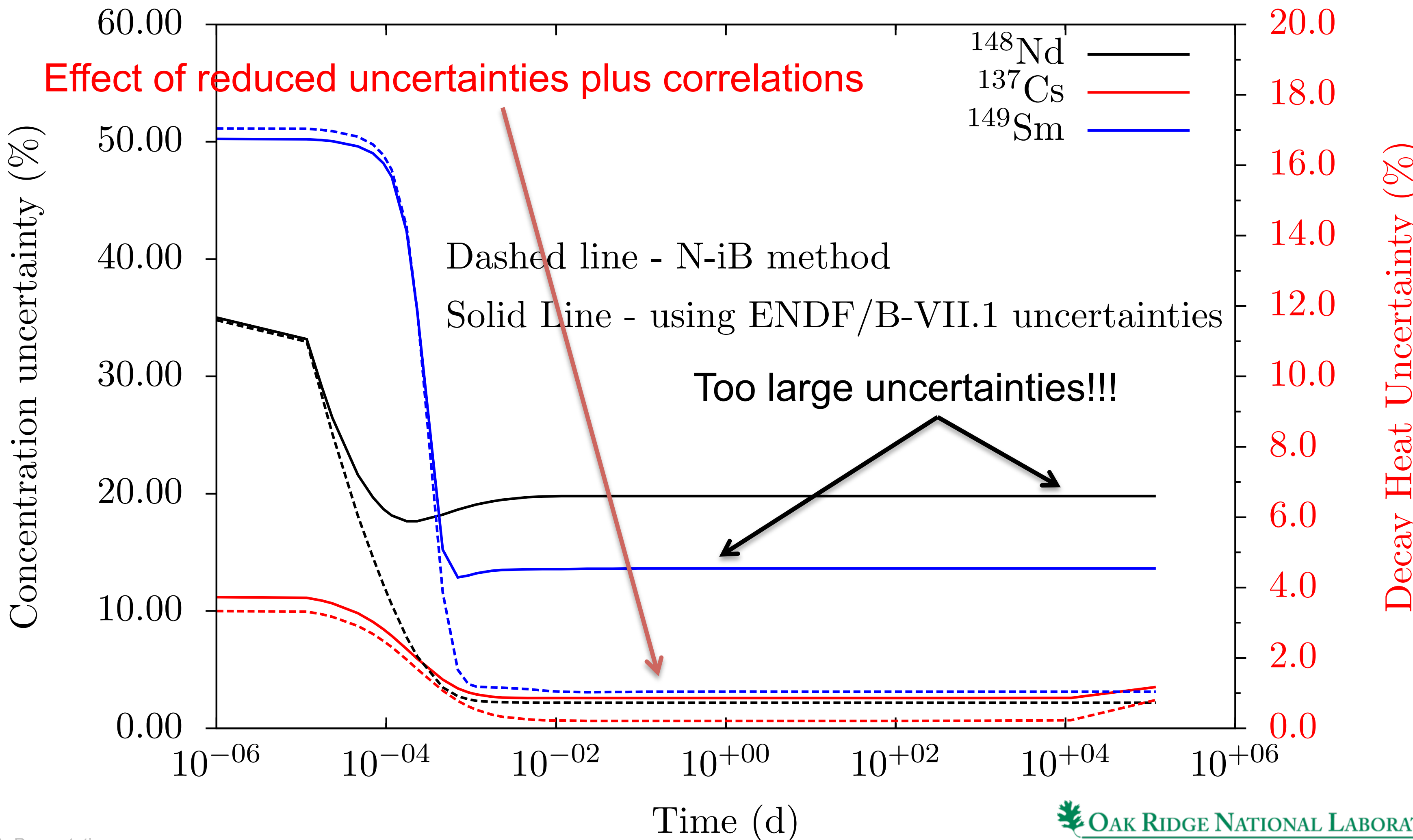
Table 2. Uncertainties and Correlation Matrix for Bayesian Adjusted Covariance File (148 Mass Chain)

				FPY Uncertainty(%)		Correlation matrix (x 100)										A = 148
Element	Z	Isotope	FPY*	Prior*	Post	Xe-148	Cs-148	Ba-148	La-148	Ce-148	Pr-148	Pr-148	Nd-148	Pm-148	Pm-148	Sm-148
1	54	Xe-148	0.109992e-10	64.00	64.00	100.0										
2	55	Cs-148	0.130991e-06	64.00	45.25	-0.006	100.0									
3	56	Ba-148	0.221844e-03	64.00	36.81	-0.000	-0.049	100.0								
4	57	La-148	0.336285e-02	64.00	40.94	-0.000	-0.001	-3.508	100.0							
5	58	Ce-148	0.123548e-01	23.00	11.28	-0.000	-0.001	-2.368	-97.48	100.0						
6	59	Pr-148m	0.388608e-03	64.00	44.79	-0.000	-0.000	-0.069	-2.823	-9.145	100.0					
7	59	Pr-148	0.388608e-03	64.00	62.67	-0.000	-0.000	-0.098	-4.034	-13.07	-2.996	100.0				
8	60	Nd-148	0.992930e-05	64.00	64.00	-0.000	-0.000	-0.002	-0.101	-0.327	-0.075	-0.107	100.0			
9	61	Pm-148	0.444969e-10	64.00	45.76	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	100.0		
10	61	Pm-148m	0.809943e-10	64.00	41.42	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-10.39	100.0	
11	62	Sm-148	0.163988e-13	64.00	64.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.003	-0.005	100.0

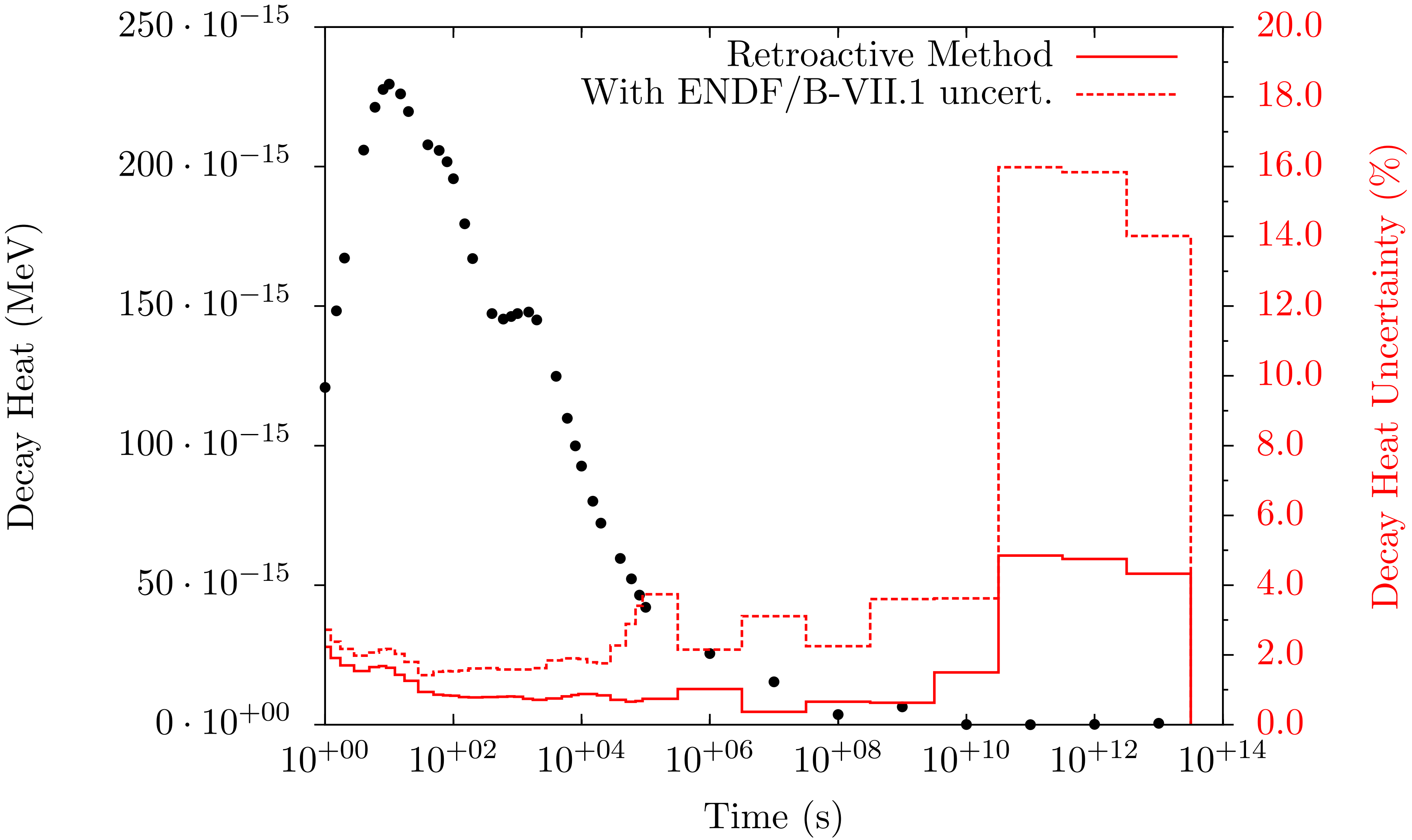
* Values are from ENDF/B-VII.0.

Change in uncertainties and correlations

Example on A=148 mass chain



Uncertainties on decay heat



SUMMARY / CONCLUSIONS

- We developed and tested methodologies to generate covariance matrices on FPY
- We developed and implemented the capability to define uncertainty distributions for fission product yields and also nuclear decay data (SAMPLER)
- 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 differences are understood by the use of different libraries or decay schemes)
  - The correlations increase on average the relative uncertainties on DH. This is understood by the fact the correlation matrix was coupled with existing uncertainties.
- On the base of isotopic concentrations we believe that uncertainties in ENDF/B-VII.1 are too large. A non-iterative Bayesian method can be used to account for the information on the cumulative: proper correlations and uncertainties are generated.