Covariance and uncertainty on fission yields: propagation to decay heat

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NEA/DB

Topical Day | From nuclear data to a reliable estimate of spent fuel decay heat
October 26, 2017 Mol (BELGIUM)

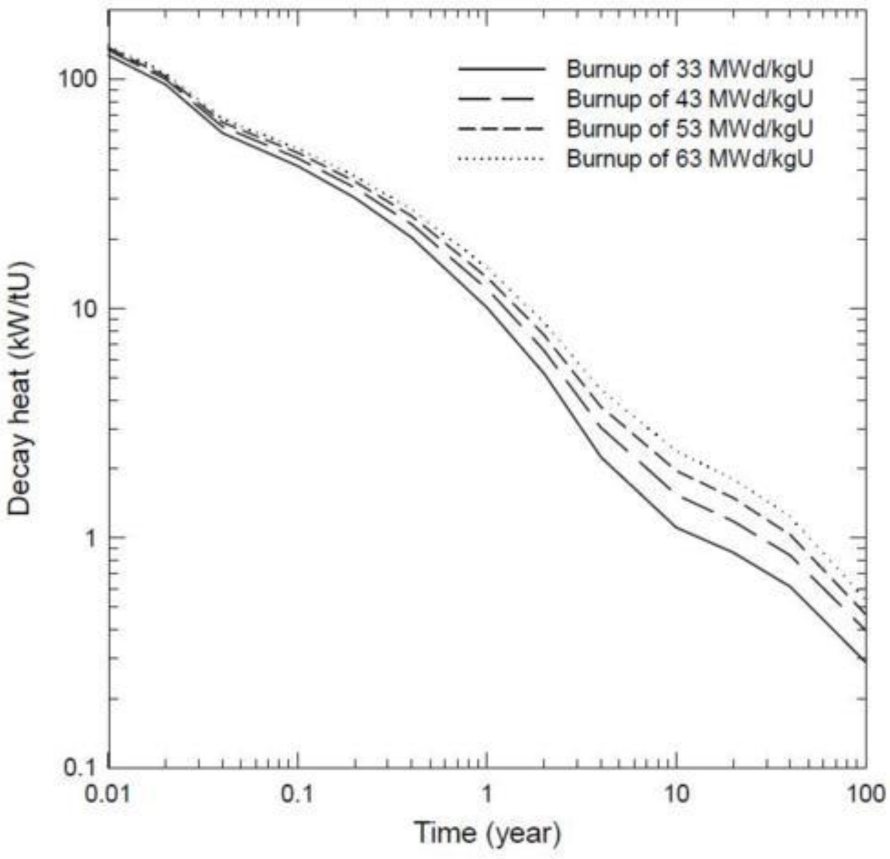
Decay heat

- What is decay heat?

  Delayed heat released from components of the nuclear system from the effect of radiation on material

  - Fuel assembly
  - Structural material
  - coolant

- Important for:
  - ☐ Reactor transient analyses
  - ☐ Reactor shutdown analyses
  - ☐ Removal of fuel from reactors
  - ☐ Storage of spent fuel
  - ☐ Transport of spent fuel
  - ☐ Reprocessing of spent fuel



Decay heat equations

- Burnup equation

$$\begin{cases} \frac{d\mathbf{n}(t)}{dt} = \mathbf{A}\mathbf{n}(t) \\ \mathbf{n}(t_{in}) = \mathbf{n}_{in} \end{cases}$$

- Reaction rate

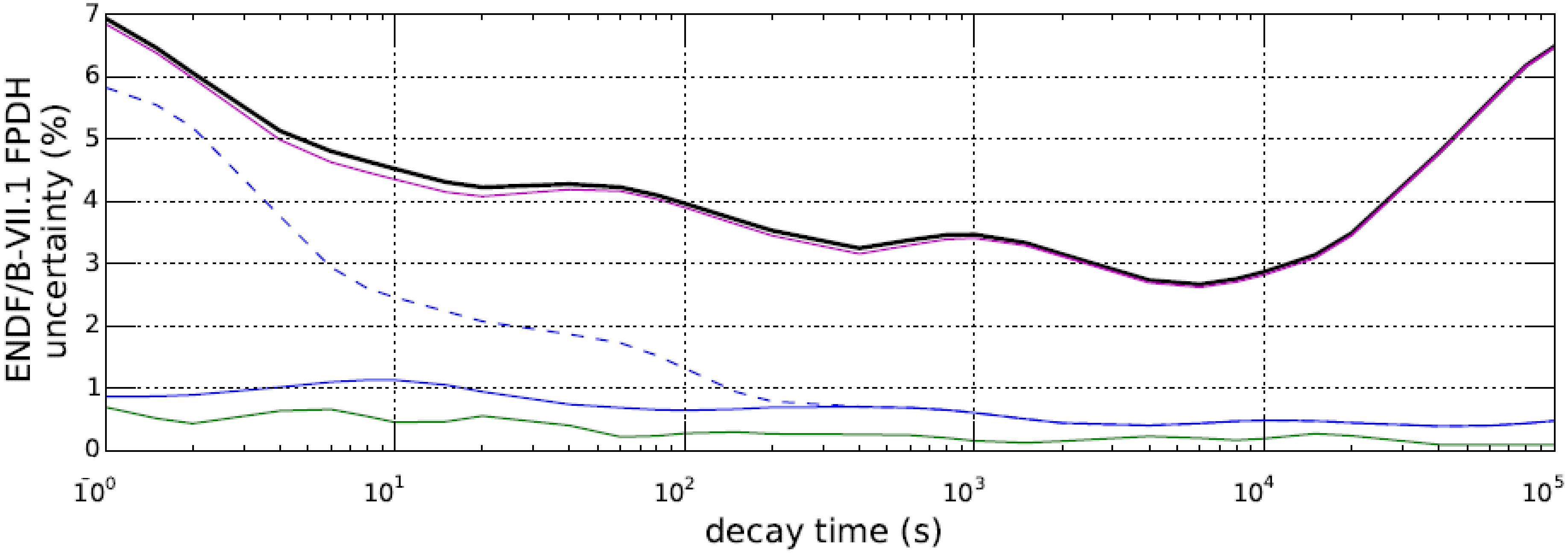
$$a_{i,j} = \lambda_j \beta_{j\to i} + \sum_{r\neq f} \int_0^\infty \sigma_{r,j}^{XS}(E)\phi(E)dE + \int_0^\infty \underline{y_{j\to i}}(E)\sigma_{f,j}^{XS}(E)\phi(E)dE$$

- Decay heat

$$DH(T) = \sum_i DH_i(T) = \sum_i \lambda_i n_i(T) E_i^d$$

  - λ: decay constant
  - n : nuclide density
  - E^d : decay energy
  - β : branching ratio
  - y : fission yield
  - σ : cross section
  - ϕ : neutron flux

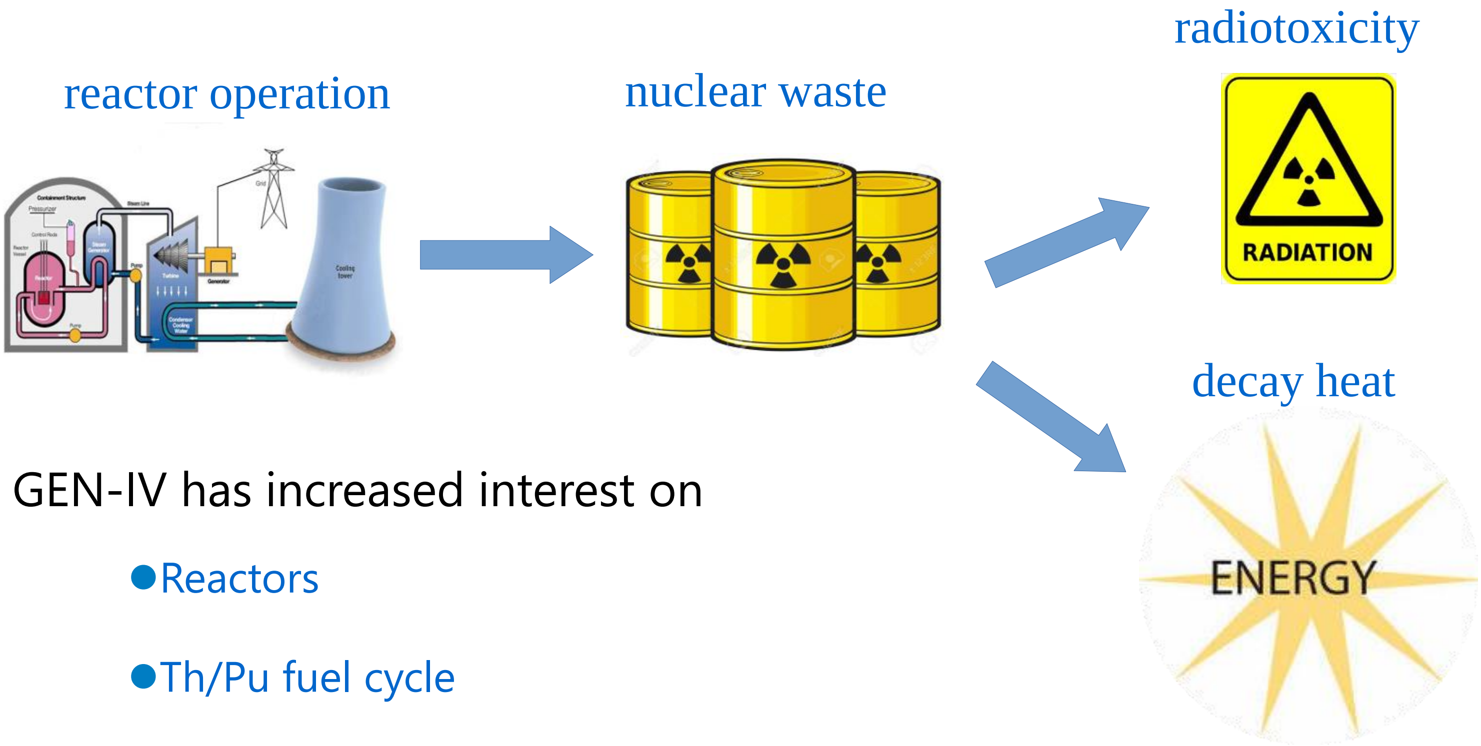
Uncertainty on decay heat



- Largest contribution comes from the fission product yields

Fission products

Fission products reduce nuclear fuel performances and are eventually considered as waste



reactor operation

nuclear waste

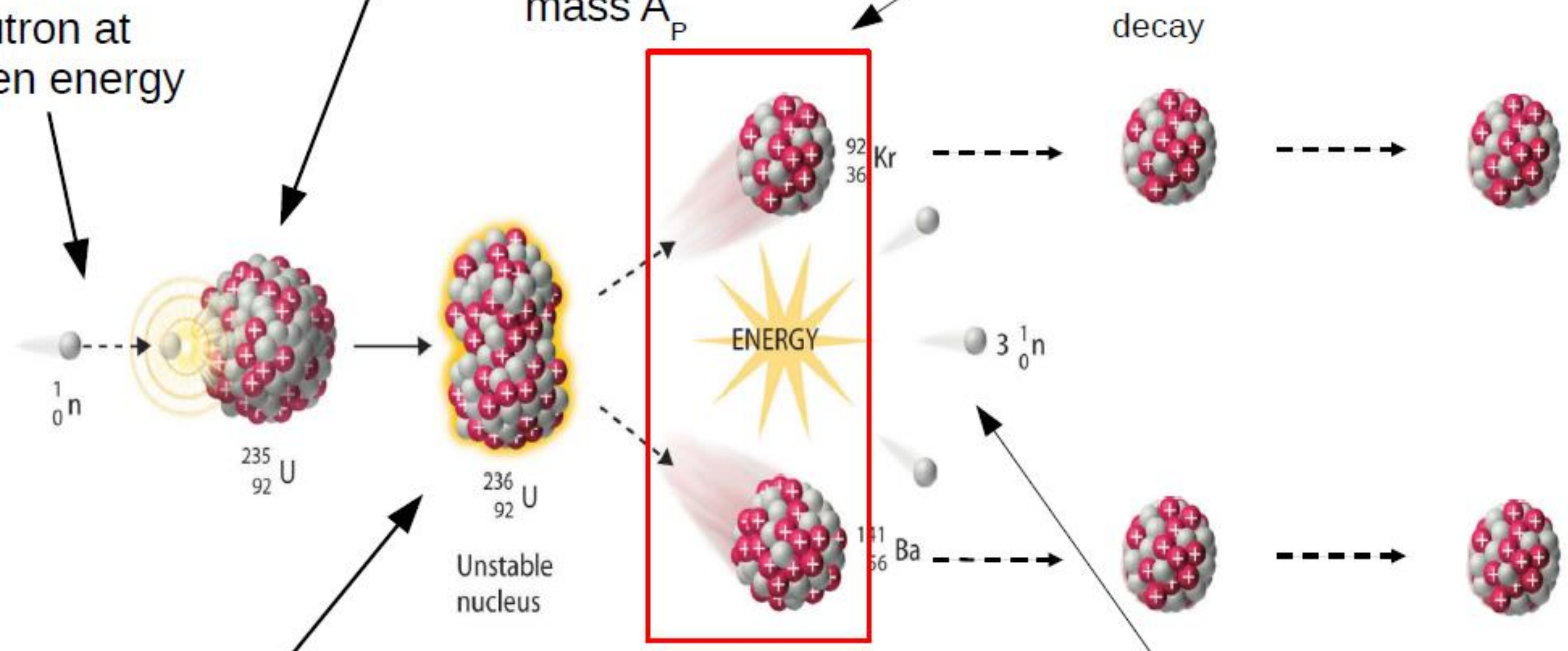
radiotoxicity

decay heat

GEN-IV has increased interest on

- Reactors
- Th/Pu fuel cycle
- P&T
- Waste management

Fission event



Incident neutron at given energy

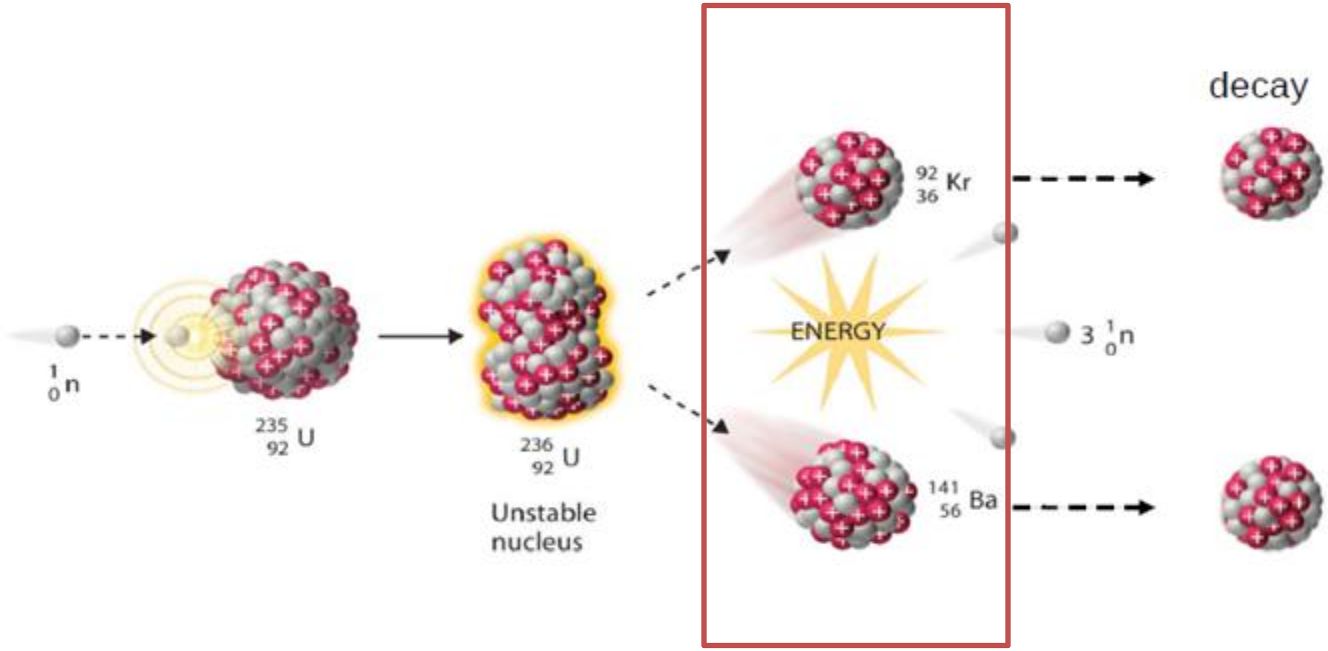
Parent nuclide: charge Z_P mass A_P

Two fission fragments

Compound nucleus: charge Z_{CN} mass $A_{CN} = A_P + 1$

Prompt neutrons

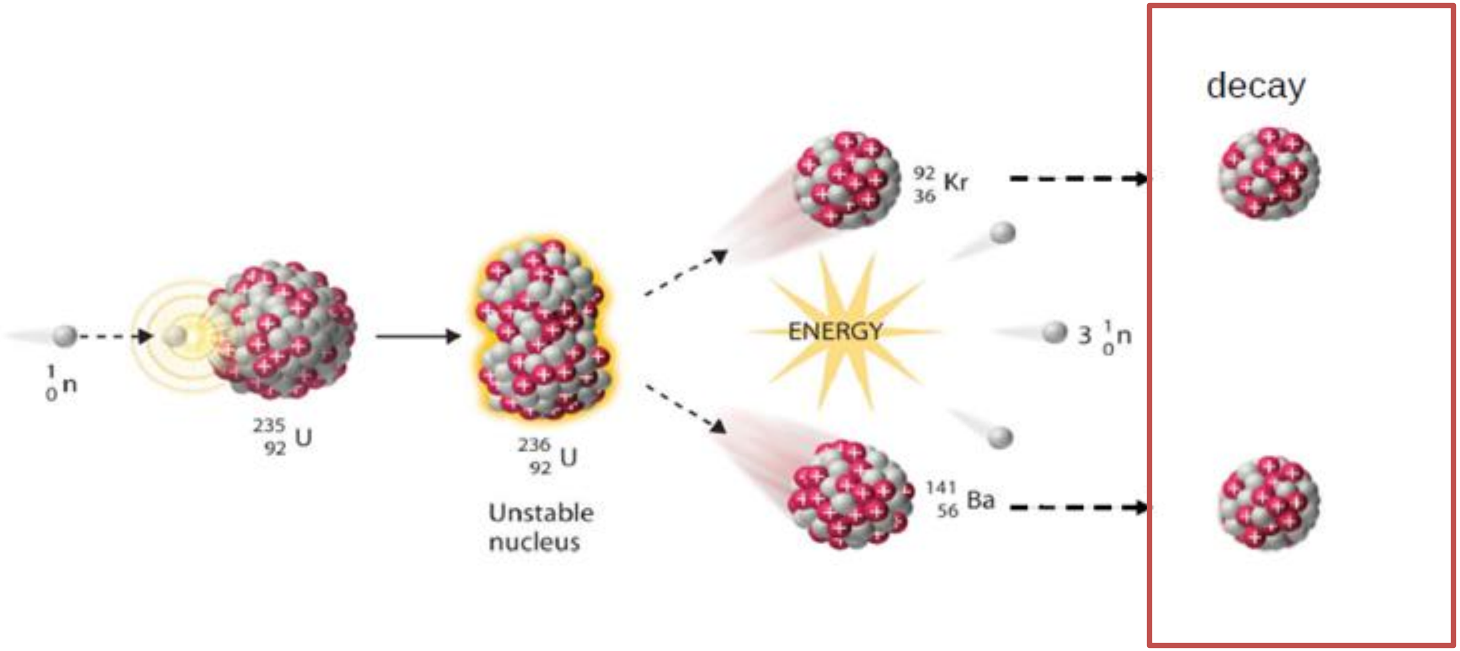
Independent fission yields (IFYs)



- **Independent fission yield:**

“atomic fraction of a specific nuclide with mass A, charge Z and metastate I, generated by a single neutron-induced fission of a given parent nuclide, after the emission of prompt neutrons and before the radioactive decay of the fission fragments”

Cumulative fission yields (CFYs)



- **Cumulative fission yield:**

“atomic fraction of a specific nuclide with mass A, charge Z and metastate I, generated by a single neutron-induced fission of a given parent nuclide and cumulated via decay of its precursors”

Current status of the fission yields

- Fission product yields in the ENDF-6 format file:
  - MF8/MT454 : independent fission yields (CFY)
  - MF8/MT459 : cumulative fission yields (CFY)
- ENDF/B, JENDL and JEFF used semi-empirical models to produce evaluated fission yields
- The new JEFF release will include evaluated fission yields produced with the GEF code

IFYs models

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

Sum yields for a mass chain A

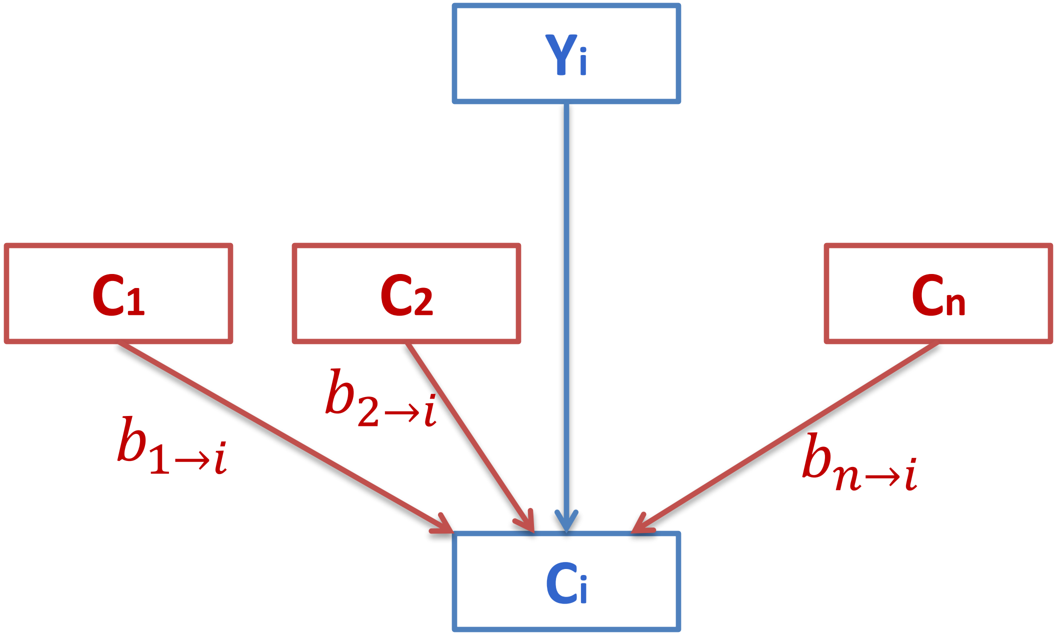
Fractional independent yields

Isomeric yield ratio

	ENDF/B-VII.1	JEFF-3.1.1	JENDL-4
$Y(A)$	Summation of Gaussian functions	Summation of Gaussian functions	Summation of Gaussian functions
$f(A,Z)$	Z_P model by Wahl + odd/even effect	Z_P model by Wahl + odd/even effect	Z_P model by Wahl + odd/even effect
$r_i(A,Z)$	Madland & England model + 50/50 split	Madland & England model	Madland & England model
Ternary yields	Not treated (Z_P model corrected)	Serot, *et. al* + UKFY3.6A	England & Rider + Mills

Derivation of CFYs

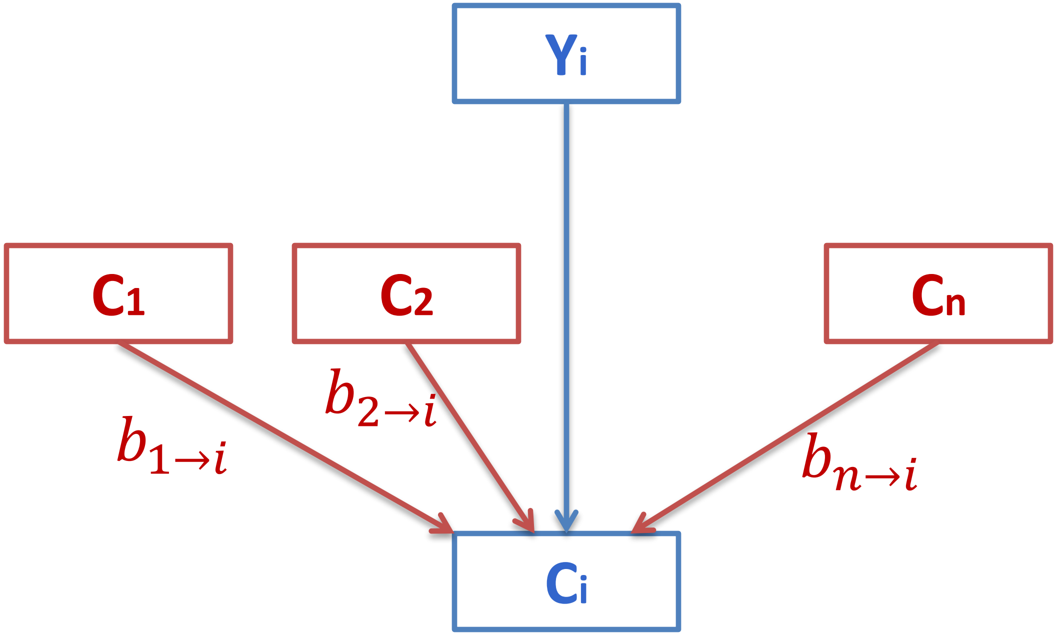
- Use the **Q-matrix** method (fission + ∞ decay time)



$$C_i = Y_i + \sum_{j \neq i} b_{j\to i} C_j \longrightarrow Y = (1 - B) C$$

Derivation of CFYs

- Use the **Q-matrix** method (fission + ∞ decay time)



- Q-matrix equation $C = QY$ where $Q = (1 - B)^{-1}$

Discrepancies on FY uncertainties

- Calculation of burnup indicators

$$N_{Nd^{148}}(t)=\frac{\Sigma_F\,\varphi\, C_{Nd^{148}}}{\sigma_c^{Nd^{148}}\,\varphi}\left(1-\exp\left(\sigma_c^{Nd^{148}}\,\varphi\, t\right)\right)$$

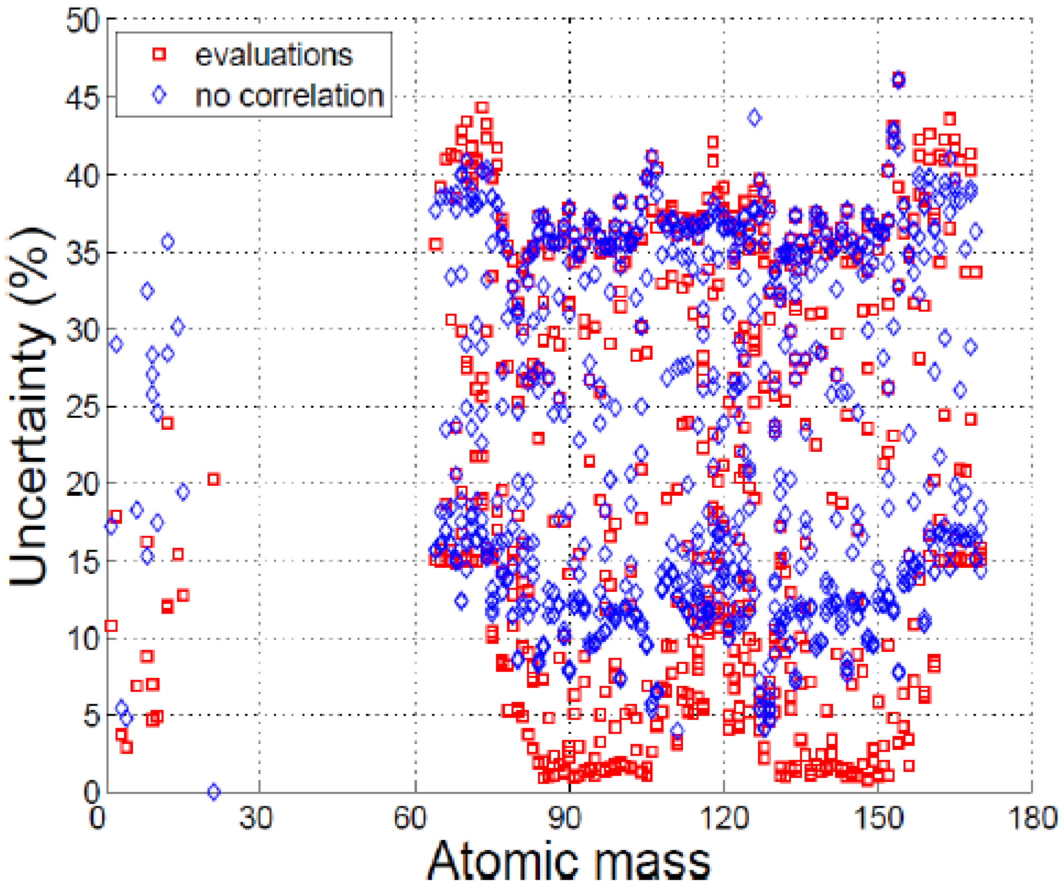
- Uncertainty propagation to Nd-148 cumulative fission yield

$$C=Q\,Y \longrightarrow V_C=Q^T V_Y\, Q$$

	JEFF-3.1.1	ENDF/B-VII.1
Evaluated	0.7%	0.35%
Calculated	9.67%	21.42%

Discrepancies on FY uncertainties

- Discrepancy on most CFYs in JEFF-3.1.1



Need for fission yield covariances

- General purpose libraries do not provide covariances for fission yields
- Institutes started producing their own covariance matrices
  - GEF (K. Schmidt)
  - GLSM (M. Pigni)
  - GLSM (N. Terranova)
  - GEF + Bayesian (D. Rochman)
  - GLSM (L. Fiorito)
  - …

Bayes method for continuous variables

- $\vec{y}$: observables
- $\vec{x}$: model parameters
- $\vec{t}(\vec{x})$: theoretical model

Multivariate prior distribution of $\vec{x}$

Likelihood function

$$p_{post}(\vec{x}\,|\,\vec{y}\,U)d\vec{x} = \frac{p_{prior}(\vec{x}\,|\,U)\mathcal{L}(\vec{y}\,|\,\vec{x}\,U)d\vec{x}}{\underbrace{\int p_{prior}(\vec{x}\,|\,U)\mathcal{L}(\vec{y}\,|\,\vec{x}\,U)d\vec{x}}}$$

Prior predictive probability $p(\vec{y})$ of the outcomes $\vec{y}$

GLSM

Principle of maximum entropy

- If $p_{prior}(\vec{x})$ is Gaussian, then

$$p_{post}(\vec{x}|\vec{y}) \propto \exp\left\{-\frac{1}{2}\left[(\vec{x}-\vec{x}_p)^{\dagger}\mathbf{C}_p^{-1}(\vec{x}-\vec{x}_p)+(\vec{y}-\vec{t}(\vec{x}))^{\dagger}\mathbf{C}_y^{-1}(\vec{y}-\vec{t}(\vec{x}))\right]\right\}$$

- How shall we derive $\vec{x}_{post}$ and $\boldsymbol{C}_{post}$ which merge both prior and new information?

$$\chi^2 = \begin{bmatrix} \vec{x}-\vec{x}_p \\ \vec{y}-\vec{t}(\vec{x}_p) \end{bmatrix}^{+} \begin{bmatrix} \boldsymbol{C}_{\boldsymbol{p}} & \boldsymbol{H} \\ \boldsymbol{H}^{+} & \boldsymbol{C}_{\boldsymbol{y}} \end{bmatrix}^{-1} \begin{bmatrix} \vec{x}-\vec{x}_p \\ \vec{y}-\vec{t}(\vec{x}_p) \end{bmatrix} = minimum$$

🟦 Prior information 🟩 New information

GLSM

- $\boldsymbol{H} = \boldsymbol{0}$ if no correlation between prior and new information

$$\chi^2 = \underbrace{\left(\vec{y} - \vec{t}(\vec{x}_p)\right)^+ \boldsymbol{C_y}^{-1}\left(\vec{y} - \vec{t}(\vec{x}_p)\right)}_{\textit{Conventional LS}} + \underbrace{\left(\vec{x} - \vec{x}_p\right)^+ \boldsymbol{C_p}^{-1}\left(\vec{x} - \vec{x}_p\right)}_{\textit{General LS}}$$

- For a linearized problem:
  - $\vec{t}(\vec{x}) \rightarrow \boldsymbol{G}\vec{x}$ where $(G)_{i,j} = \left(\frac{\partial t_i}{\partial x_j}\right)$
  - $\boldsymbol{K} = \boldsymbol{C_p}\boldsymbol{G}^+\left(\boldsymbol{G}\boldsymbol{C_p}\boldsymbol{G}^+ + \boldsymbol{C_y}\right)^{-1}$

- Prior information
- New information

$$\boxed{\begin{aligned} \vec{x}_{post} &= \vec{x}_p + \boldsymbol{K}\left(\vec{y} - \vec{t}(\vec{x}_p)\right) \\ \boldsymbol{C_{post}} &= \boldsymbol{C_p} - \boldsymbol{K}\boldsymbol{G}\boldsymbol{C_p} \end{aligned}}$$

Updating process

Constrained LS

- Nuclear parameters are constrained by physical phenomena
  - Total xs equals the sum of the partial xs
  - Probability distributions are normalized to 1
  - …
- Constraining model : $\boldsymbol{G}\vec{x}_p = Q$

▪ Constraint

- $\boldsymbol{K} = \boldsymbol{C}_p \boldsymbol{G}^+ \left(\boldsymbol{G}\boldsymbol{C}_p\boldsymbol{G}^+ \cancel{+ \boldsymbol{C}_y}\right)^{-1}$

$$\chi^2{}_c = \underbrace{\left(Q - \boldsymbol{R}\vec{x}_p\right)^+ \left(\boldsymbol{R}\boldsymbol{C}_p\boldsymbol{R}^+\right)^{-1}\left(Q - \boldsymbol{R}\vec{x}_p\right)}_{\textit{Constrained LS}}$$

Constrained LS

- The updating process does not change

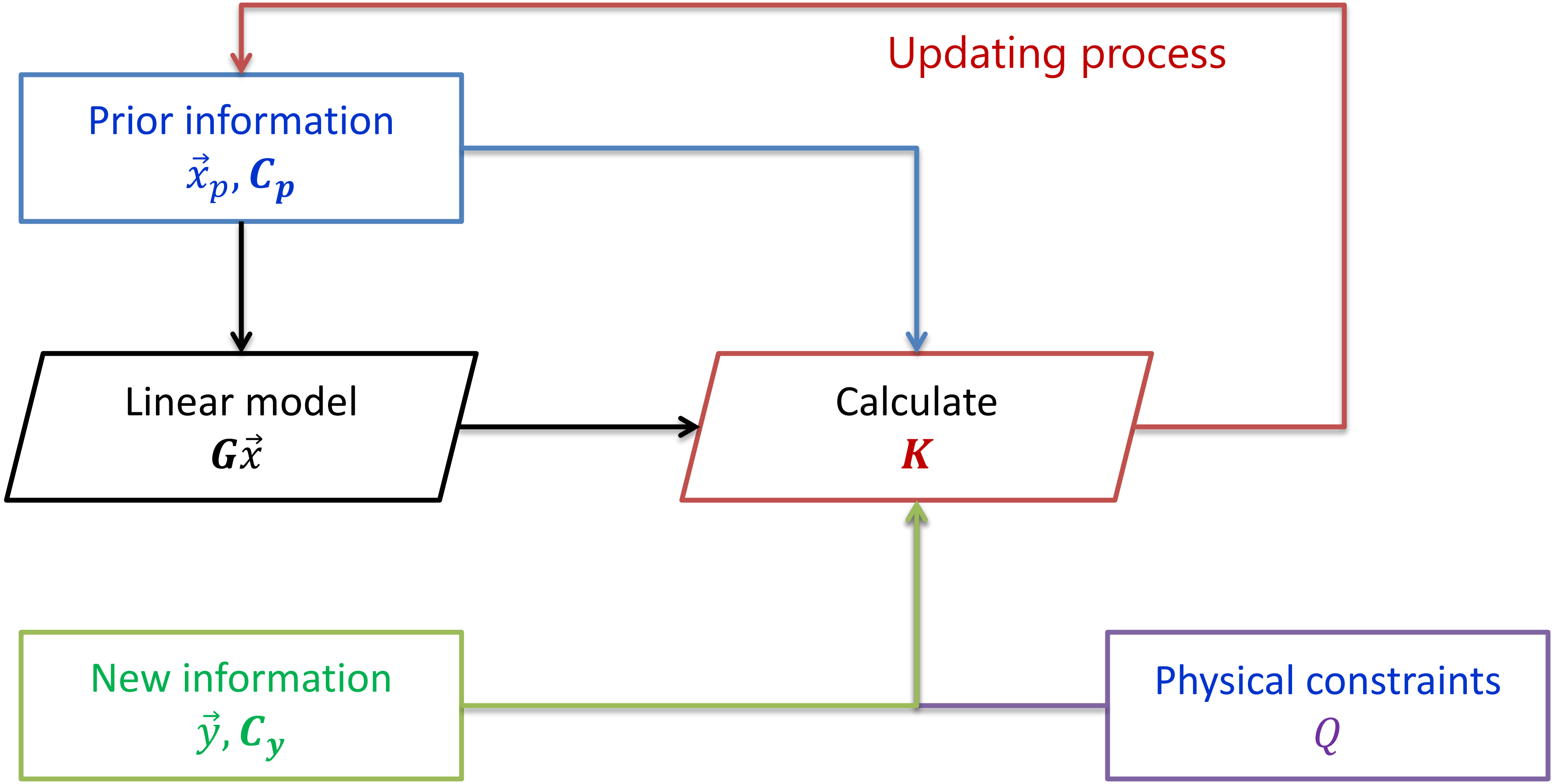
$$\boxed{\begin{aligned}\vec{x}_{post} &= \vec{x}_p + \boldsymbol{K}\left(Q - \boldsymbol{R}\vec{x}_p\right)\\ \boldsymbol{C}_{\boldsymbol{post}} &= \boldsymbol{C}_{\boldsymbol{p}} - \boldsymbol{K}\boldsymbol{G}\boldsymbol{C}_{\boldsymbol{p}}\end{aligned}}$$

Updating process

- “Constrained” cost function

$$\chi^2{}_c = \underbrace{\left(Q - \boldsymbol{R}\vec{x}_p\right)^+ (\boldsymbol{R}\boldsymbol{C}_{\boldsymbol{p}}\boldsymbol{R}^+)^{-1}\left(Q - \boldsymbol{R}\vec{x}_p\right)}_{\textit{Constrained LS}}$$

Iterative GLS update



Updating process

Prior information
$\vec{x}_p, \boldsymbol{C_p}$

Linear model
$\boldsymbol{G}\vec{x}$

Calculate
$\boldsymbol{K}$

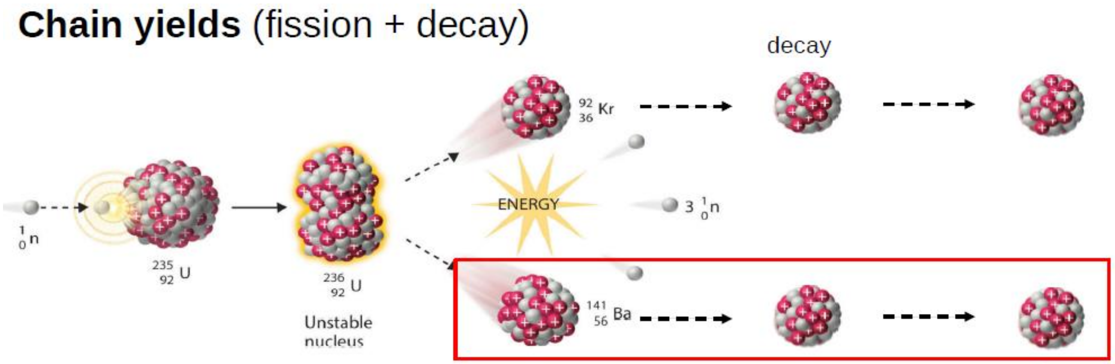
New information
$\vec{y}, \boldsymbol{C_y}$

Physical constraints
Q

SCK-CEN covariances

GLSM specifications

- **Prior information:** JEFF-3.1.1 independent fission yields + variances
- **New information:**
  - Physical constraints (x5)
  - Experimental chain fission yield (ChFY), only variances
- **Non-model update**



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- **New information:**
  - Physical constraints (x5)
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L. Fiorito, A. Stankovskiy, G. Van den Eynde, C.J. Diez, O. Cabellos, P.E. Labeau, Generation of fission yield covariances to correct discrepancies in the nuclear data libraries, In Annals of Nuclear Energy, Volume 88, 2016, Pages 12-23, ISSN 0306-4549

L. Fiorito, C.J. Diez, O. Cabellos, A. Stankovskiy, G. Van den Eynde, P.E. Labeau, Fission yield covariance generation and uncertainty propagation through fission pulse decay heat calculation, In Annals of Nuclear Energy, Volume 69, 2014, Pages 331-343, ISSN 0306-4549

FYs conservation equations

Charge conservation

$$\sum_i Z_i Y_i = Z_{CN} - Z_{LCP}$$

Mass conservation

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}_p(E) - A_{LCP}$$

Conservation of number of fragments

$$\sum_i Y_i = 2$$

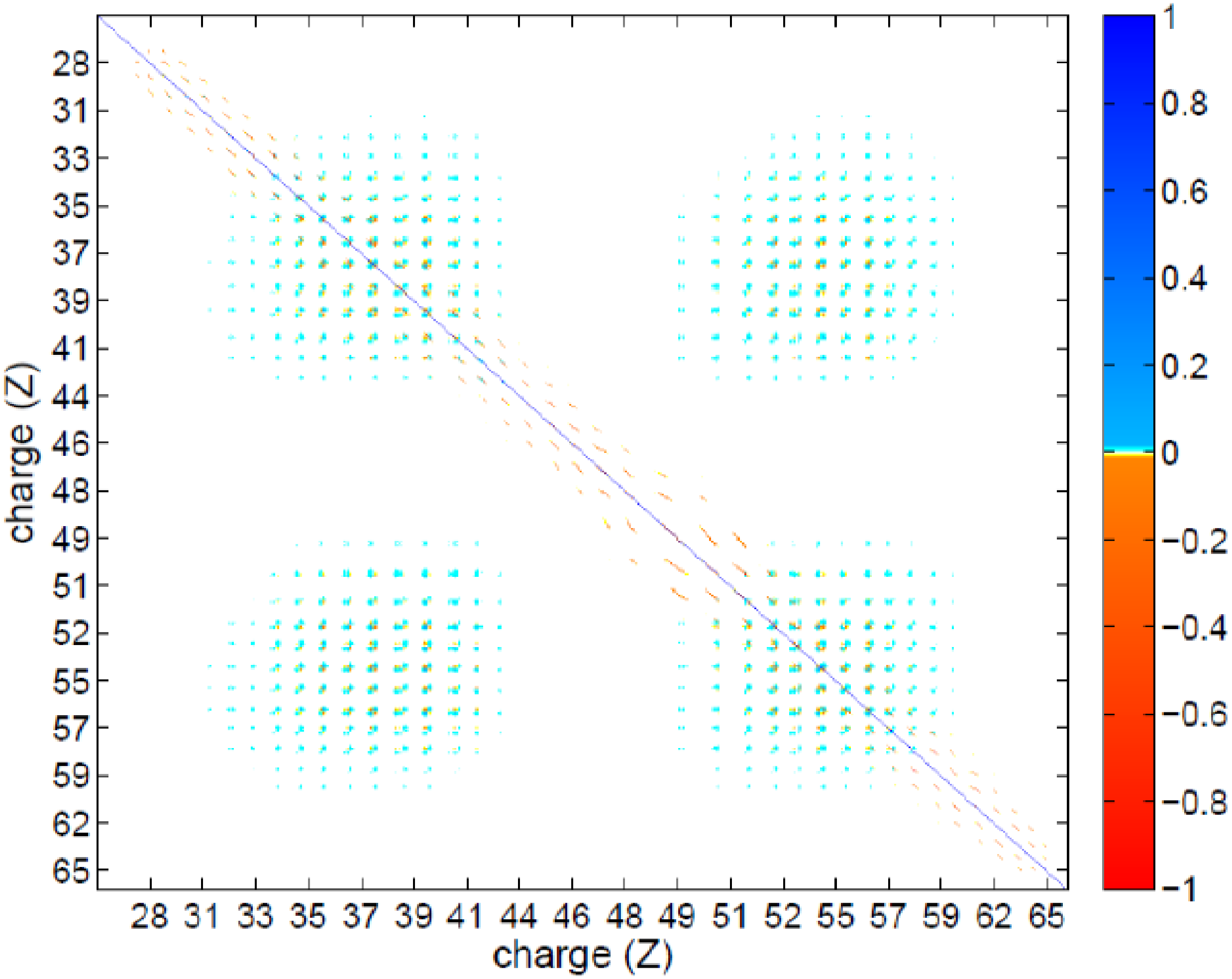
Fission asymmetry

$$\sum_{A_i > \frac{A_{CN} - \bar{\nu}_p}{2}} Y(A_i) = 1$$

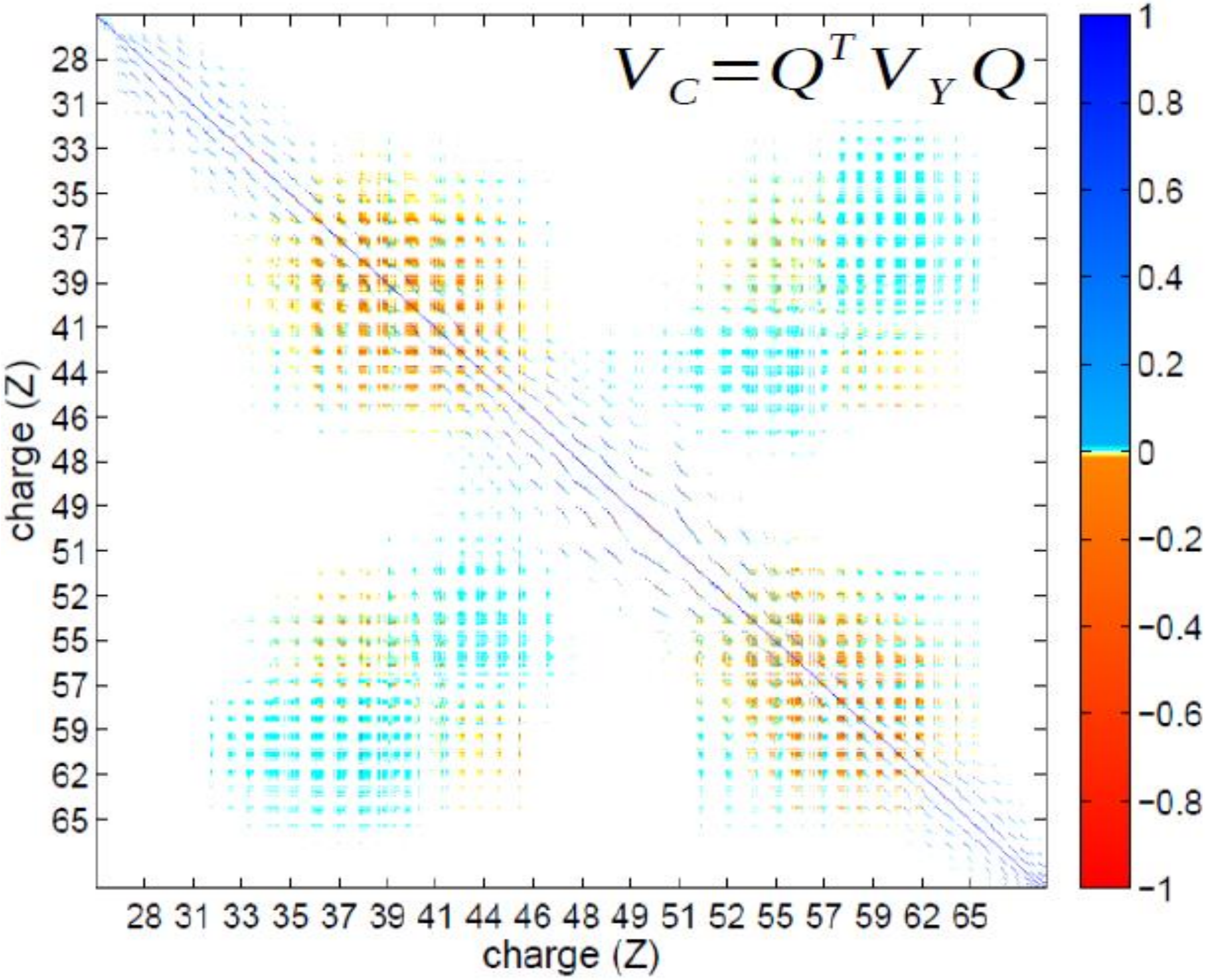
Individual charge constraints

$$\sum_{Z_i = Z'} Y(Z_i) = \sum_{Z_j = Z_{CN} - Z'} Y(Z_j)$$

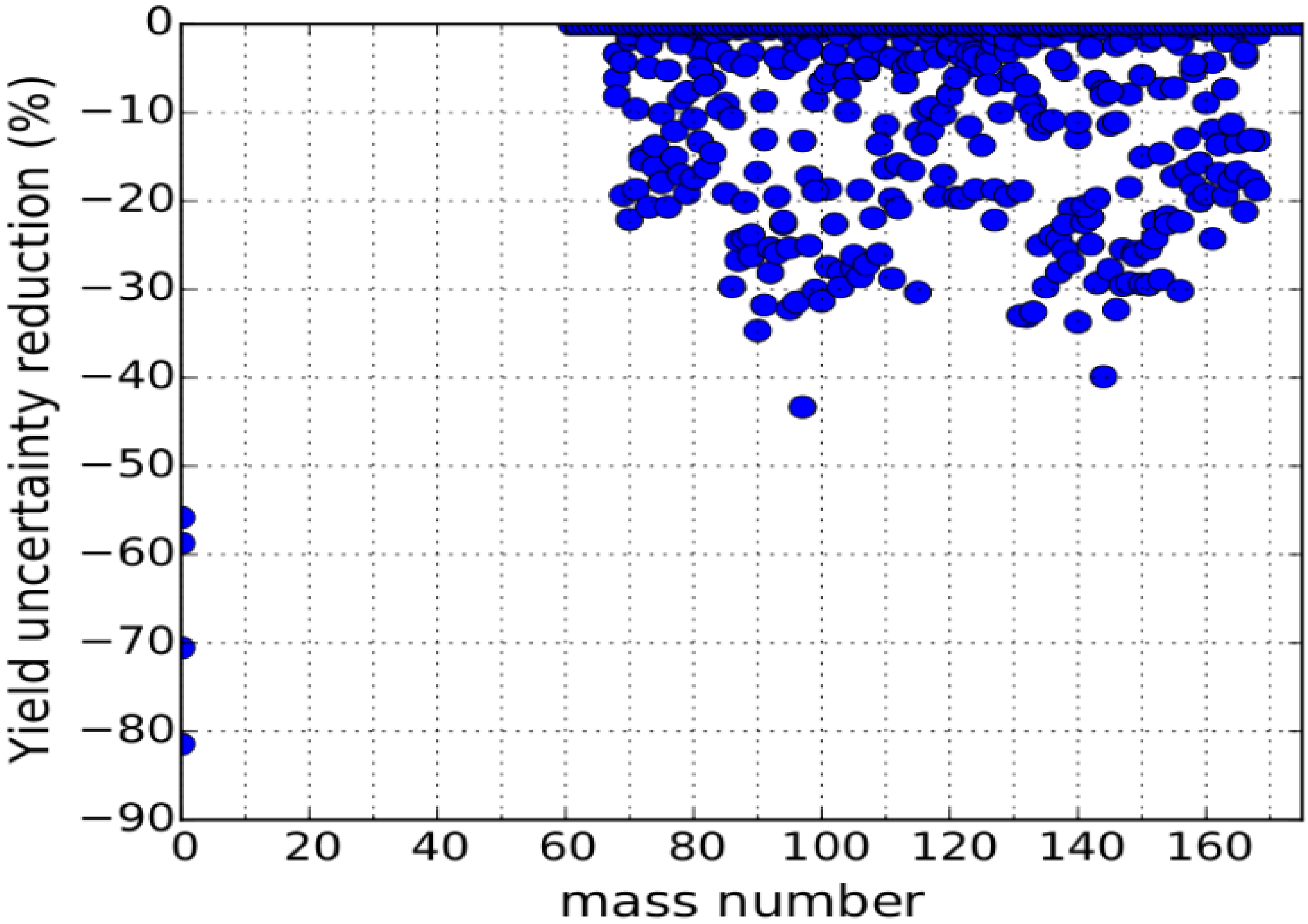
IFY covariance matrix (U-235-thermal)



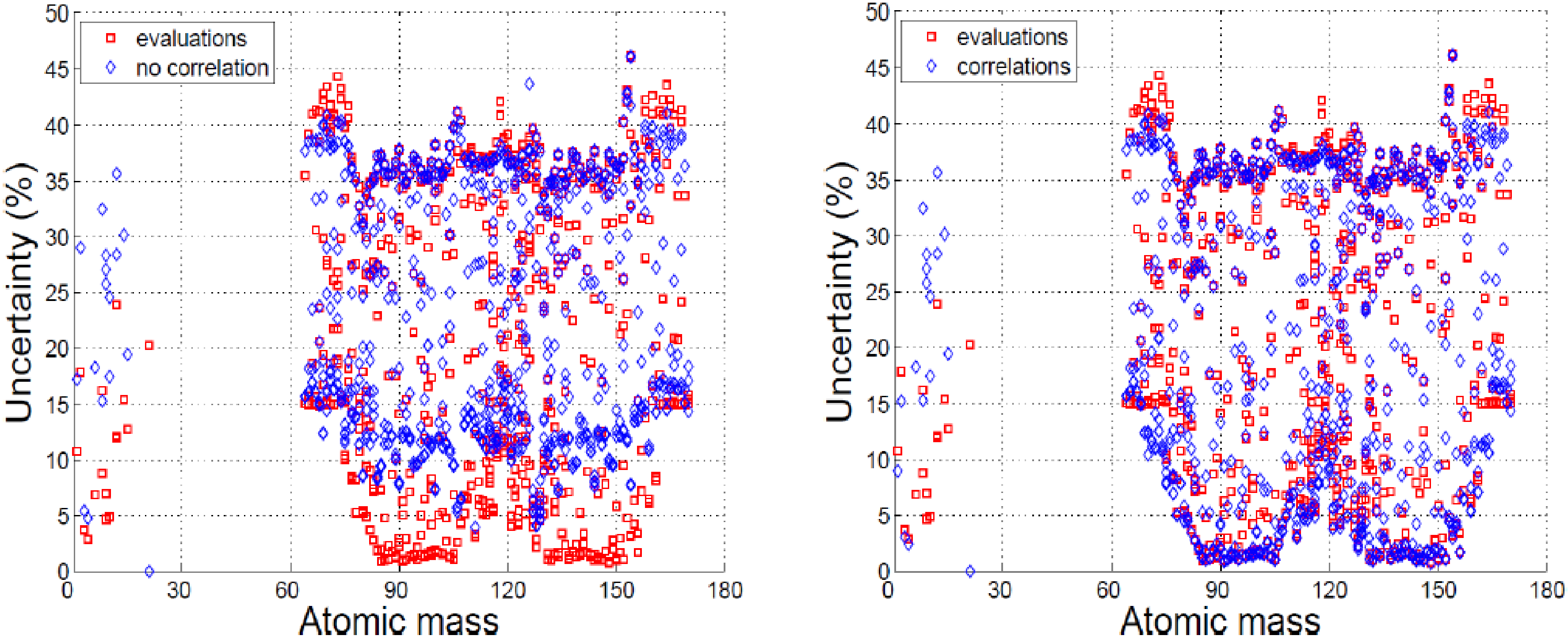
CFY covariance matrix (U-235-thermal)



IFY uncertainty reduction

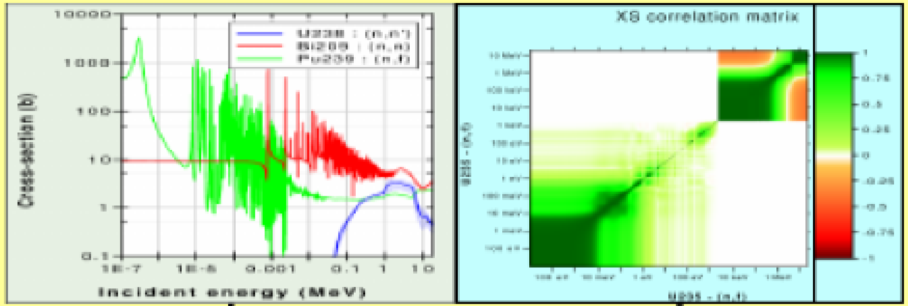


Discrepancies on FY uncertainties



Nd-148 CFY	JEFF-3.1.1	ENDF/B-VII.1
Evaluated	0.7%	0.35%
Calculated w/o COV	9.67%	21.42%
Calculated with COV	1.01%	0.35%

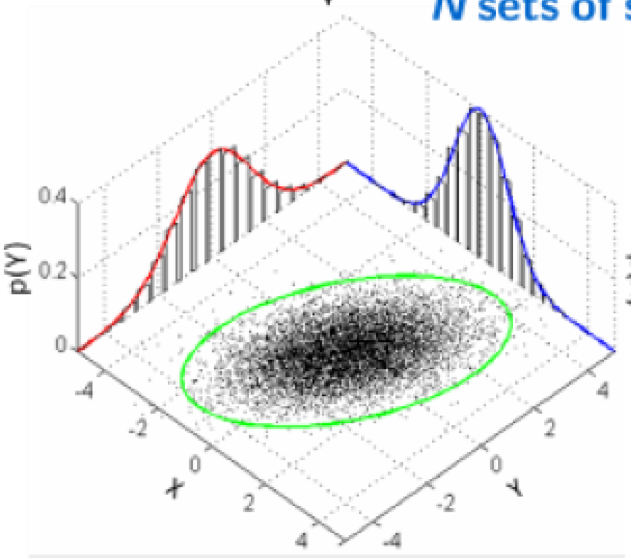
Monte Carlo sampling



ENDF-6:

- best-estimates
- covariance

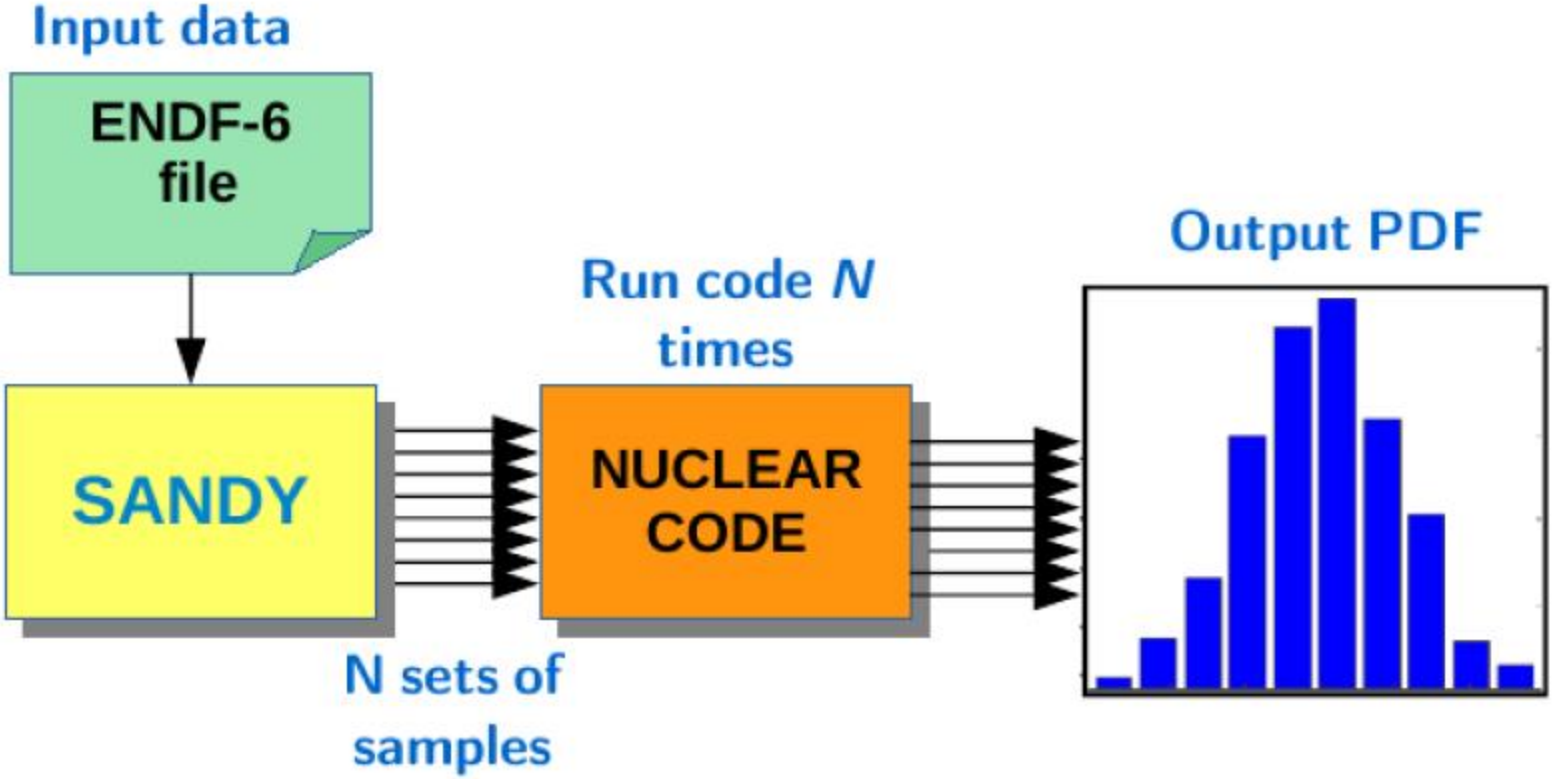
N sets of samples



Multivariate input PDF

- Sample all covariance in ENDF-6
- Apply conservation equations
- Write data in ENDF-6 format files

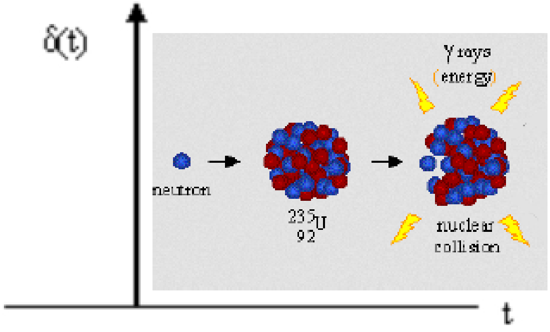
Uncertainty propagation



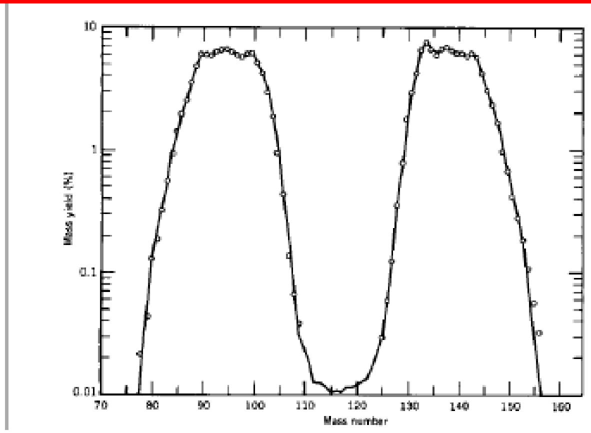
L. Fiorito, G. Žerovnik, A. Stankovskiy, G. Van den Eynde, P.E. Labeau, Nuclear data uncertainty propagation to integral responses using SANDY, In Annals of Nuclear Energy, Volume 101, 2017, Pages 359-366, ISSN 0306-4549

Fission pulse decay heat (FPDH)

INSTANTANEOUS FISSION EVENT



FISSION YIELD DISTRIBUTION



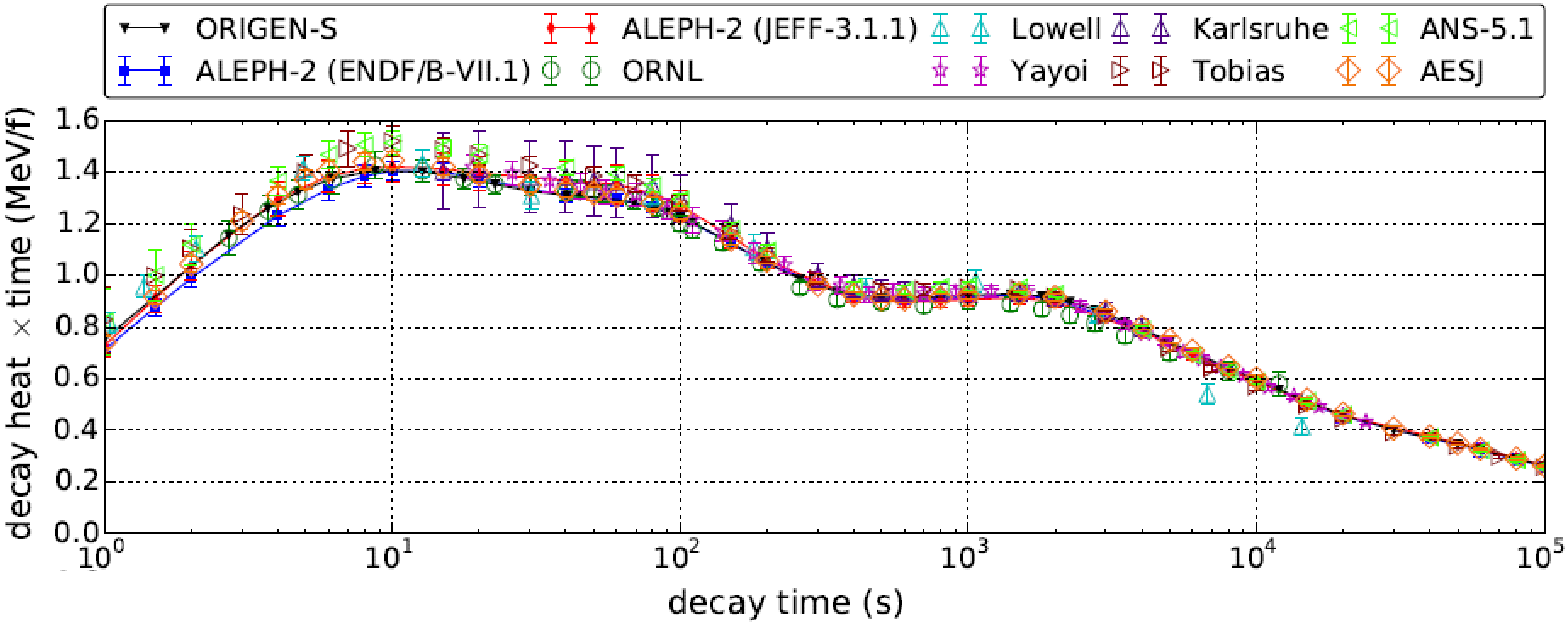
DEPLETION AND DECAY HEAT EQUATIONS

$$\begin{cases} \frac{dn_i(t)}{dt} = -\lambda_i n_i(t) + \sum_j \lambda_j \beta_{j\to i} n_j(t) \\ n_i(t=0) = \boxed{y_i} \end{cases}$$

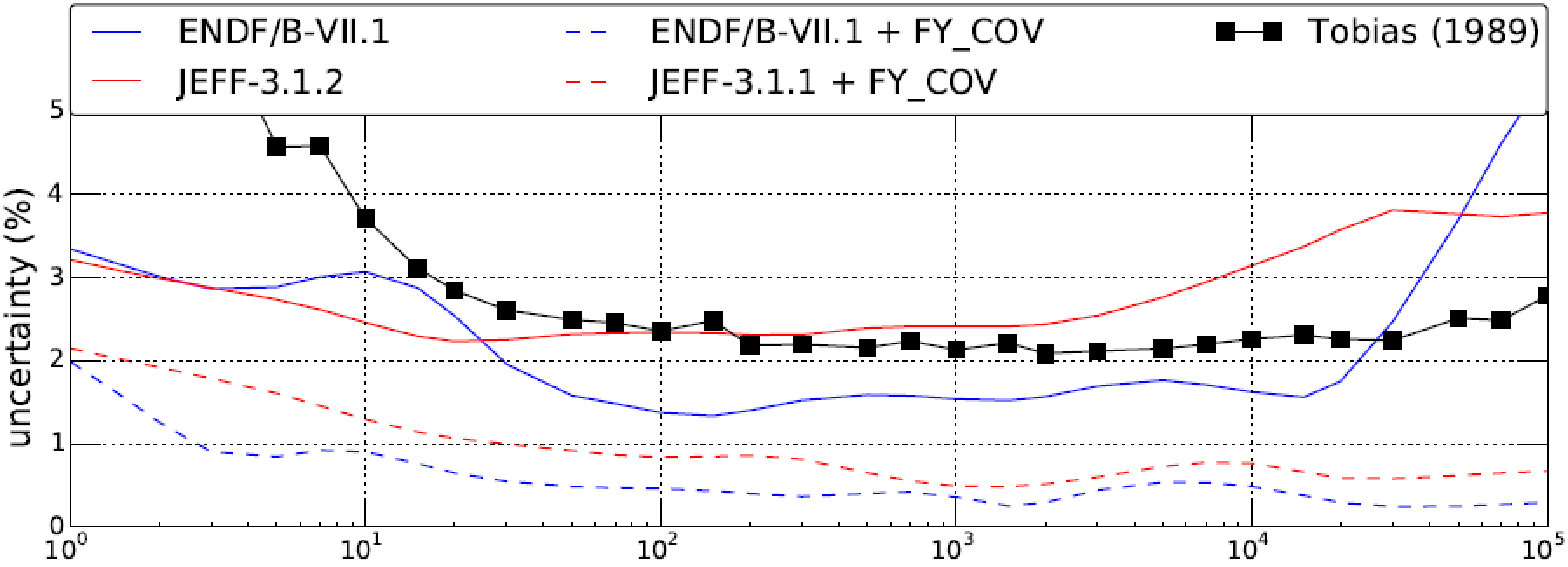
$$DH(T) = \sum_i DH_i(T) = \sum_i \lambda_i n_i(T) E_i^d$$

Fission pulse decay heat (FPDH)

- U-235 thermal fission

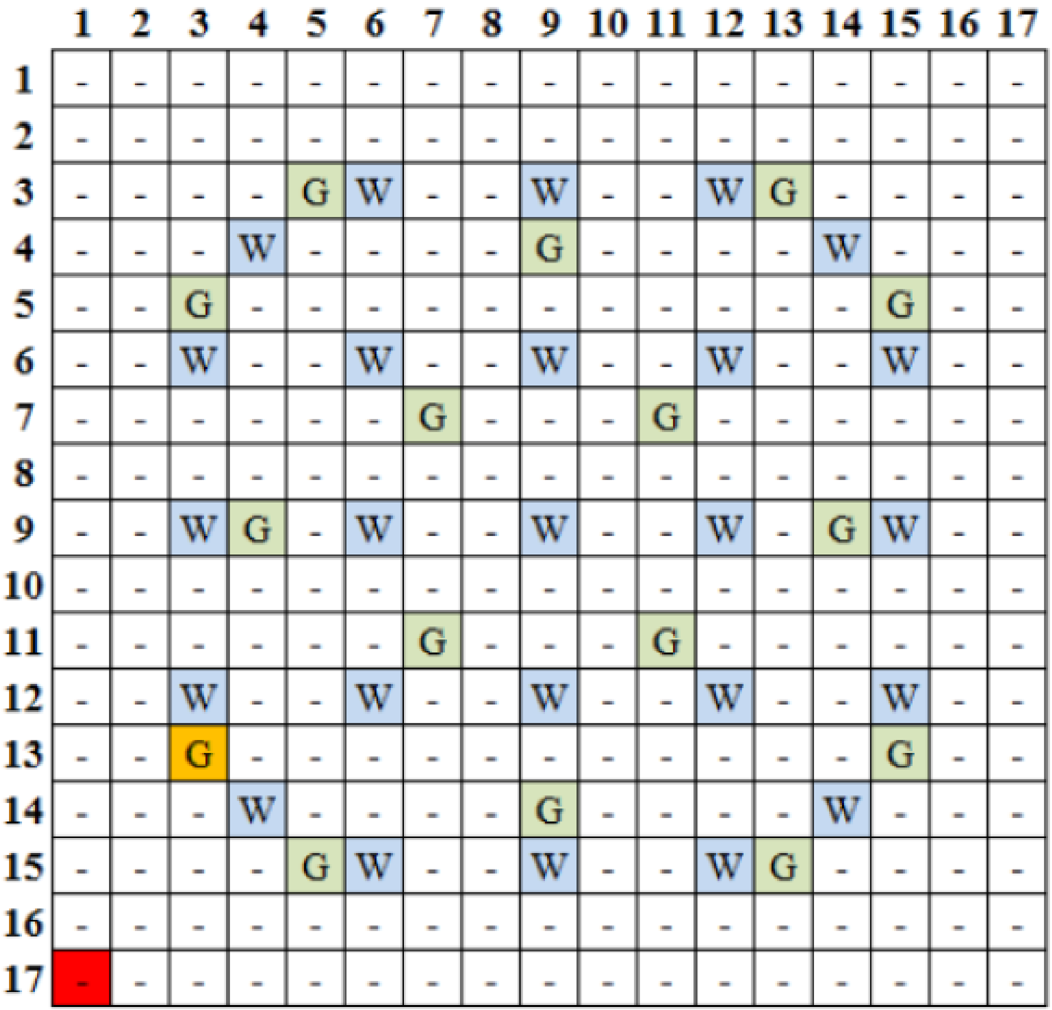


Impact on U-235 thermal FPDH



- Large reduction of the fission yield uncertainty contribution

Takahama-3 fuel assembly



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3	-	-	-	-	G	W	-	-	W	-	-	W	G	-	-	-	-
4	-	-	-	W	-	-	-	-	G	-	-	-	-	W	-	-	-
5	-	-	G	-	-	-	-	-	-	-	-	-	-	-	G	-	-
6	-	-	W	-	-	W	-	-	W	-	-	W	-	-	W	-	-
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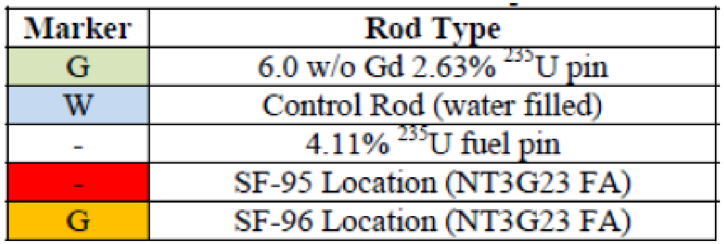


Marker	Rod Type
🟩 G	6.0 w/o Gd 2.63% ^{235}U pin
🟦 W	Control Rod (water filled)
-	4.11% ^{235}U fuel pin
🟥 -	SF-95 Location (NT3G23 FA)
🟧 G	SF-96 Location (NT3G23 FA)

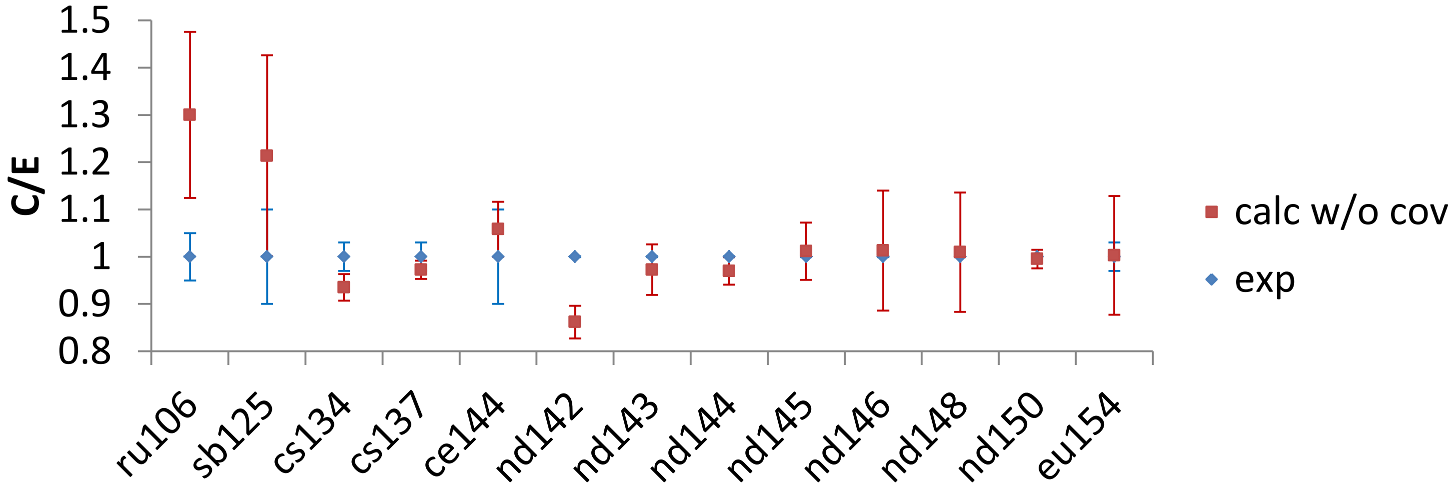
- **Cutting positions of the samples**

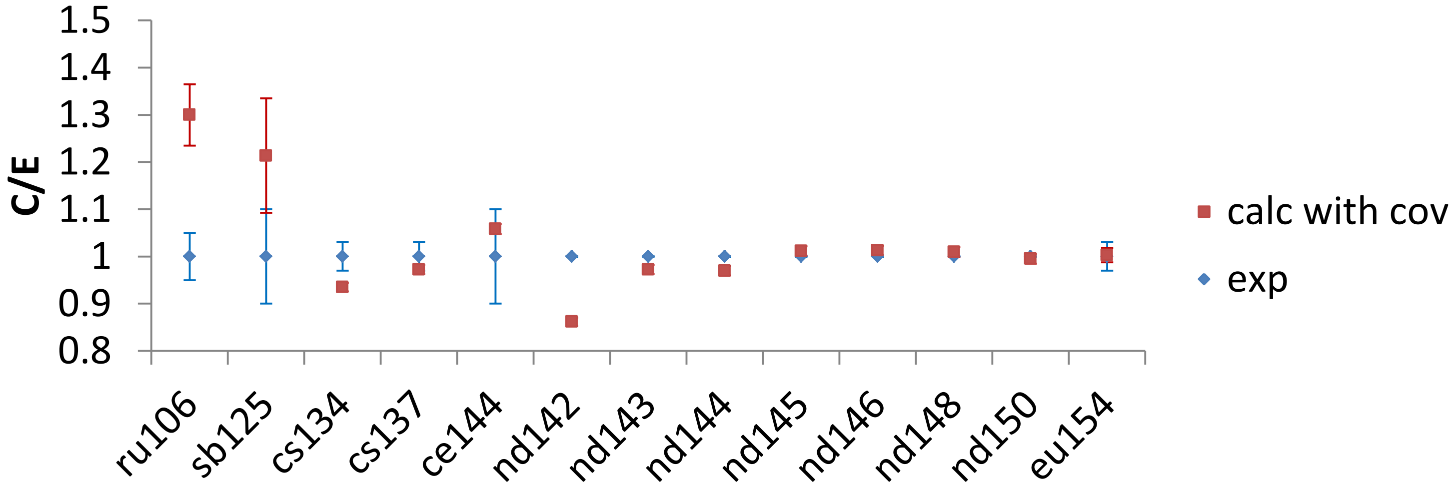
Sample ID	*From bottom of active length (mm)*
SF95-4	1646
SF96-4	1671

- **Initial isotopic composition of the fuel rods**

Isotopes	*SF95 (wt%)*	*SF96 (wt%)*
234U	0.04	0.02
235U	4.11	2.63
238U	95.85	97.25

Impact on burnup problems





Other methodologies

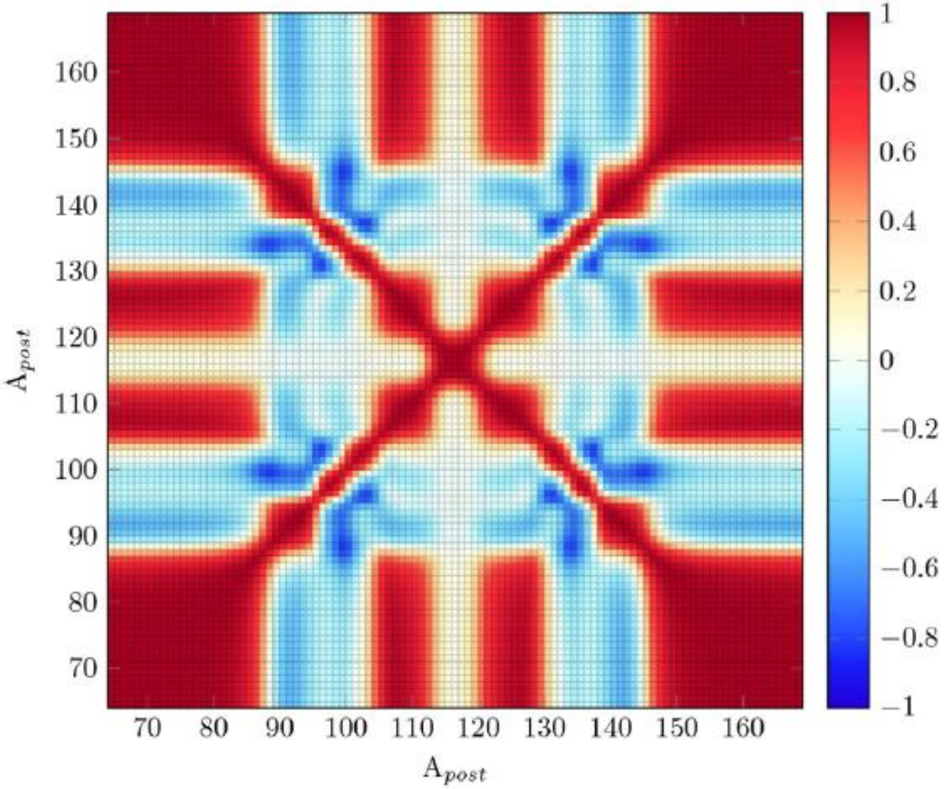
GLSM specifications

- **Prior information:**
  - model parameters taken from the literature (~20)
- **New information:**
  - Experimental miscellaneous fission quantities
  - JEFF-3.1.1 independent fission yields
- **Models:**
  - Brosa 5-Gaussian model
  - Wahl model
  - Madland and England model

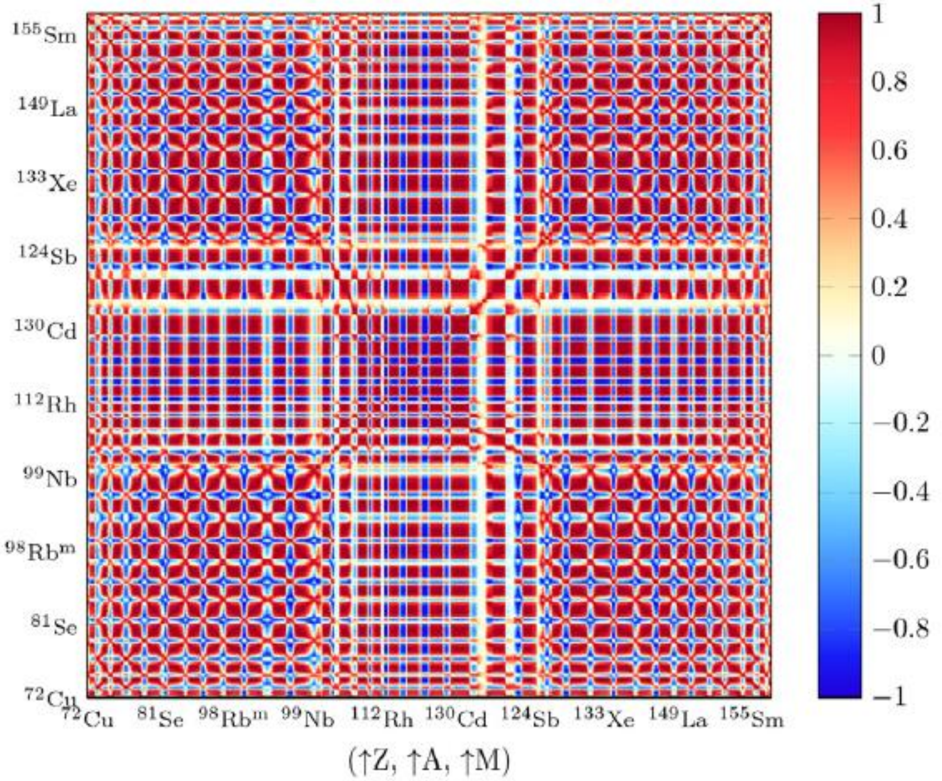
N. Terranova, O. Serot, P. Archier, C. De Saint Jean, M. Sumini, Fission yield covariance matrices for the main neutron-induced fissioning systems contained in the JEFF-3.1.1 library, In Annals of Nuclear Energy, Volume 109, 2017, Pages 469-489, ISSN 0306-4549

Correlation matrices

MFY correlation matrix

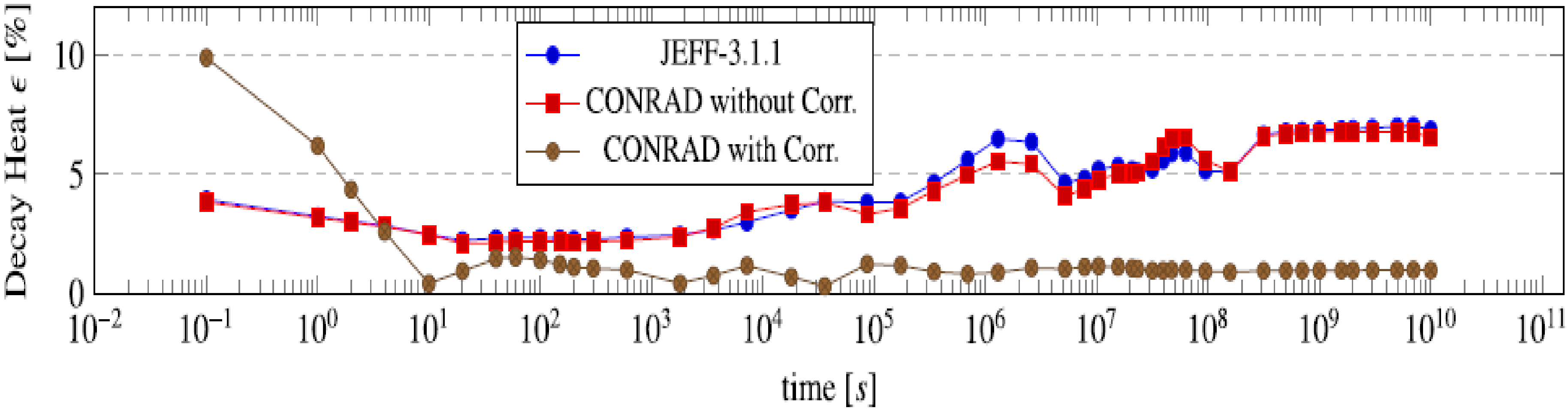


Isomeric FY correlation matrix



- Introduced marginalization effects

Impact on U-235 thermal FPDH



- Large reduction of the fission yield uncertainty contribution

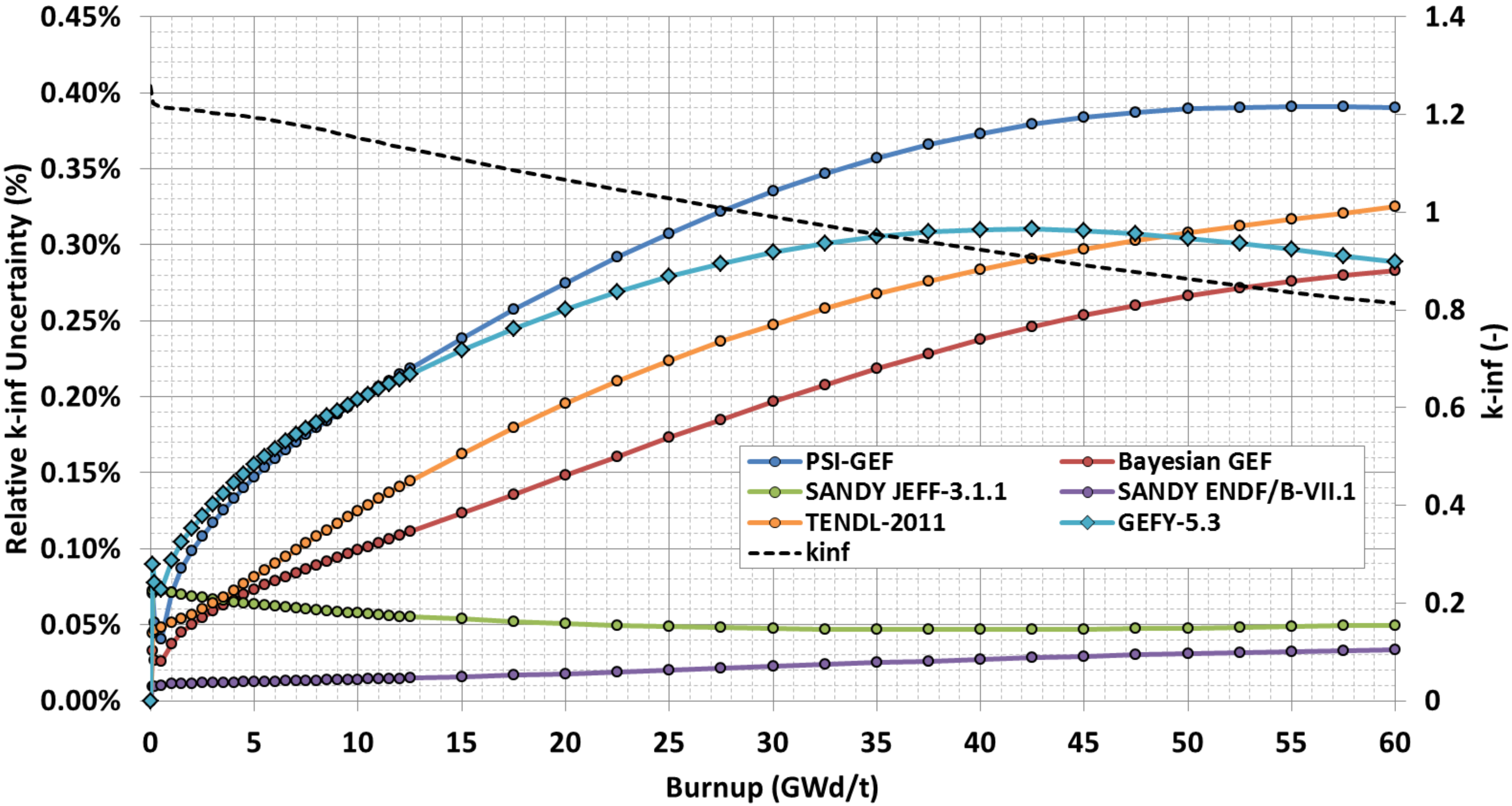
Other methodologies

- Random sampling of GEF input parameters
- Bayesian Monte Carlo + GEF

Fission yield covariances for JEFF: A Bayesian Monte Carlo method, Olivier Leray, Dimitri Rochman, Michael Fleming, Jean-Christophe Sublet, Arjan Koning, Alexander Vasiliev, Hakim Ferroukhi, EPJ Web Conf. 146 09023 (2017)

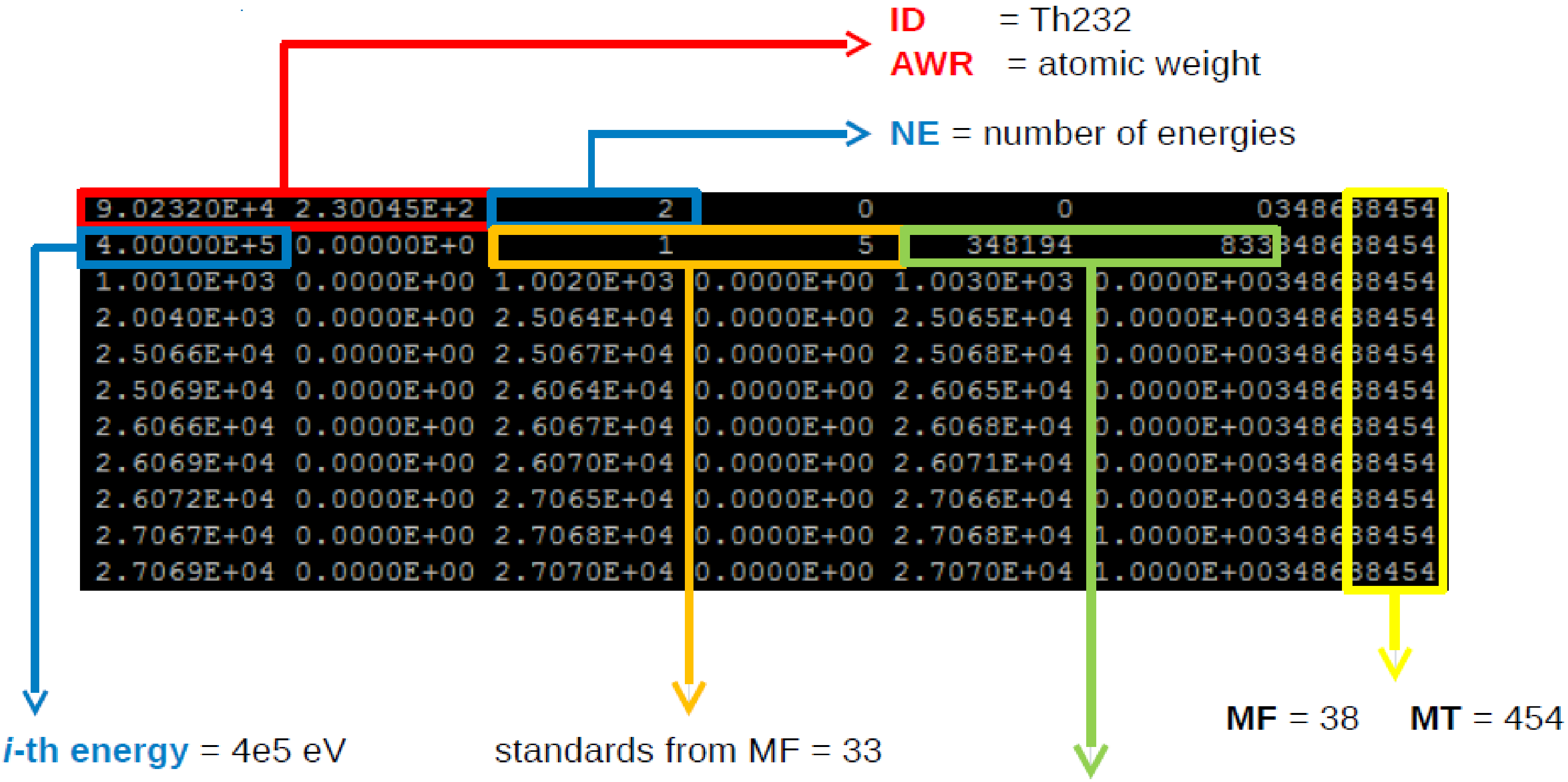
O. Leray, L. Fiorito, D. Rochman, H. Ferroukhi, A. Stankovskiy, G. Van den Eynde, Uncertainty propagation of fission product yields to nuclide composition and decay heat for a PWR UO2 fuel assembly, In Progress in Nuclear Energy, 2017, , ISSN 0149-1970

Impact on keff calculations



Need for format

- Proposed MF38 format for ENDF-6



```
 9.02320E+4 2.30045E+2          2          0          0          0348638454
 4.00000E+5 0.00000E+0          1          5     348194        833348638454
 1.0010E+03 0.0000E+00 1.0020E+03 0.0000E+00 1.0030E+03 0.0000E+00348638454
 2.0040E+03 0.0000E+00 2.5064E+04 0.0000E+00 2.5065E+04 0.0000E+00348638454
 2.5066E+04 0.0000E+00 2.5067E+04 0.0000E+00 2.5068E+04 0.0000E+00348638454
 2.5069E+04 0.0000E+00 2.6064E+04 0.0000E+00 2.6065E+04 0.0000E+00348638454
 2.6066E+04 0.0000E+00 2.6067E+04 0.0000E+00 2.6068E+04 0.0000E+00348638454
 2.6069E+04 0.0000E+00 2.6070E+04 0.0000E+00 2.6071E+04 0.0000E+00348638454
 2.6072E+04 0.0000E+00 2.7065E+04 0.0000E+00 2.7066E+04 0.0000E+00348638454
 2.7067E+04 0.0000E+00 2.7068E+04 0.0000E+00 2.7068E+04 1.0000E+00348638454
 2.7069E+04 0.0000E+00 2.7070E+04 0.0000E+00 2.7070E+04 1.0000E+00348638454
```

ID = Th232
AWR = atomic weight

NE = number of energies

***i*-th energy** = 4e5 eV

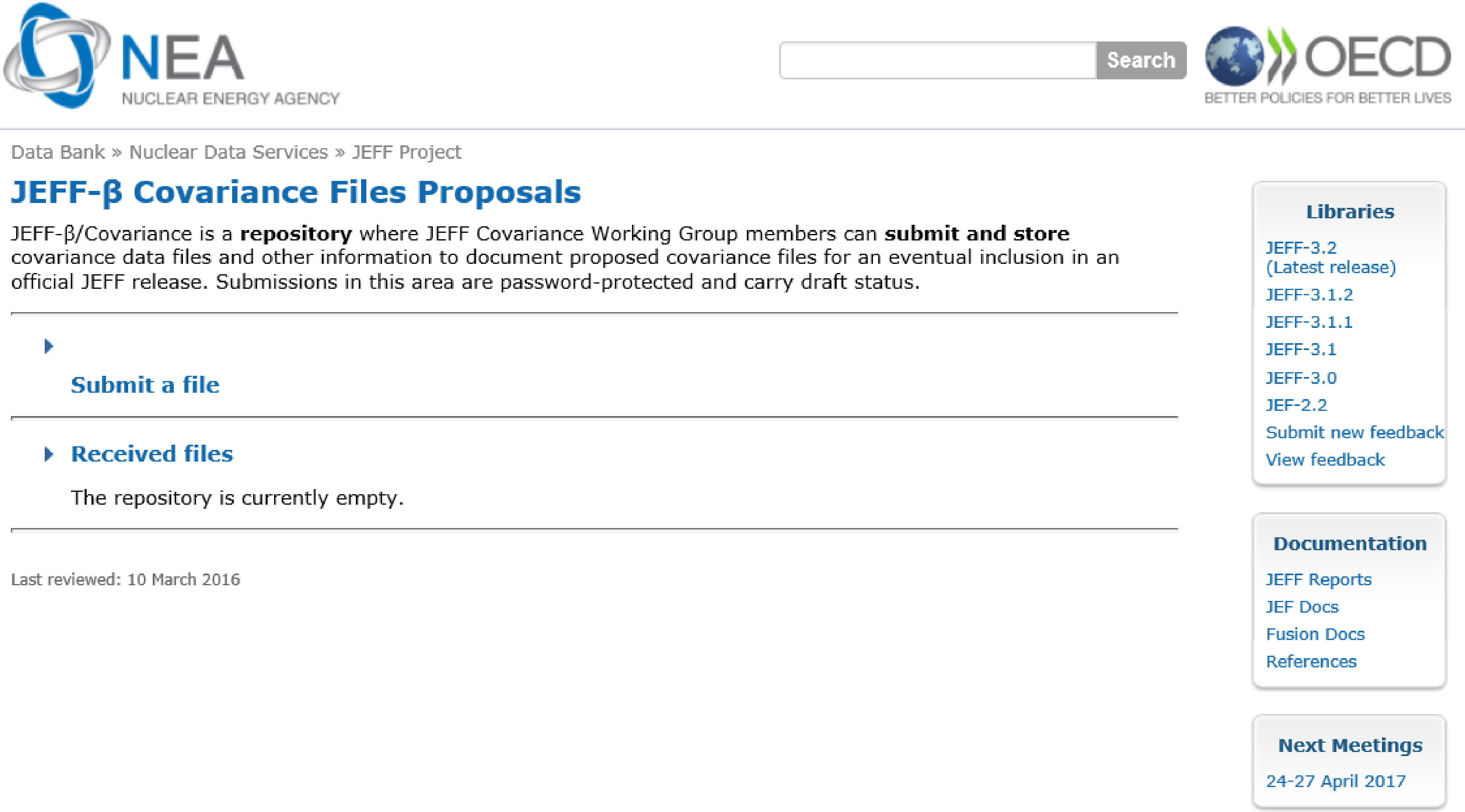
standards from MF = 33

MF = 38 **MT** = 454

NP = # stored covariance values + NFY
NFY = # of correlated yields

GND?

NEA proposed actions



Data Bank » Nuclear Data Services » JEFF Project

JEFF-β Covariance Files Proposals

JEFF-β/Covariance is a **repository** where JEFF Covariance Working Group members can **submit and store** covariance data files and other information to document proposed covariance files for an eventual inclusion in an official JEFF release. Submissions in this area are password-protected and carry draft status.

Submit a file

Received files

The repository is currently empty.

Last reviewed: 10 March 2016

Libraries

- JEFF-3.2 (Latest release)
- JEFF-3.1.2
- JEFF-3.1.1
- JEFF-3.1
- JEFF-3.0
- JEF-2.2
- Submit new feedback
- View feedback

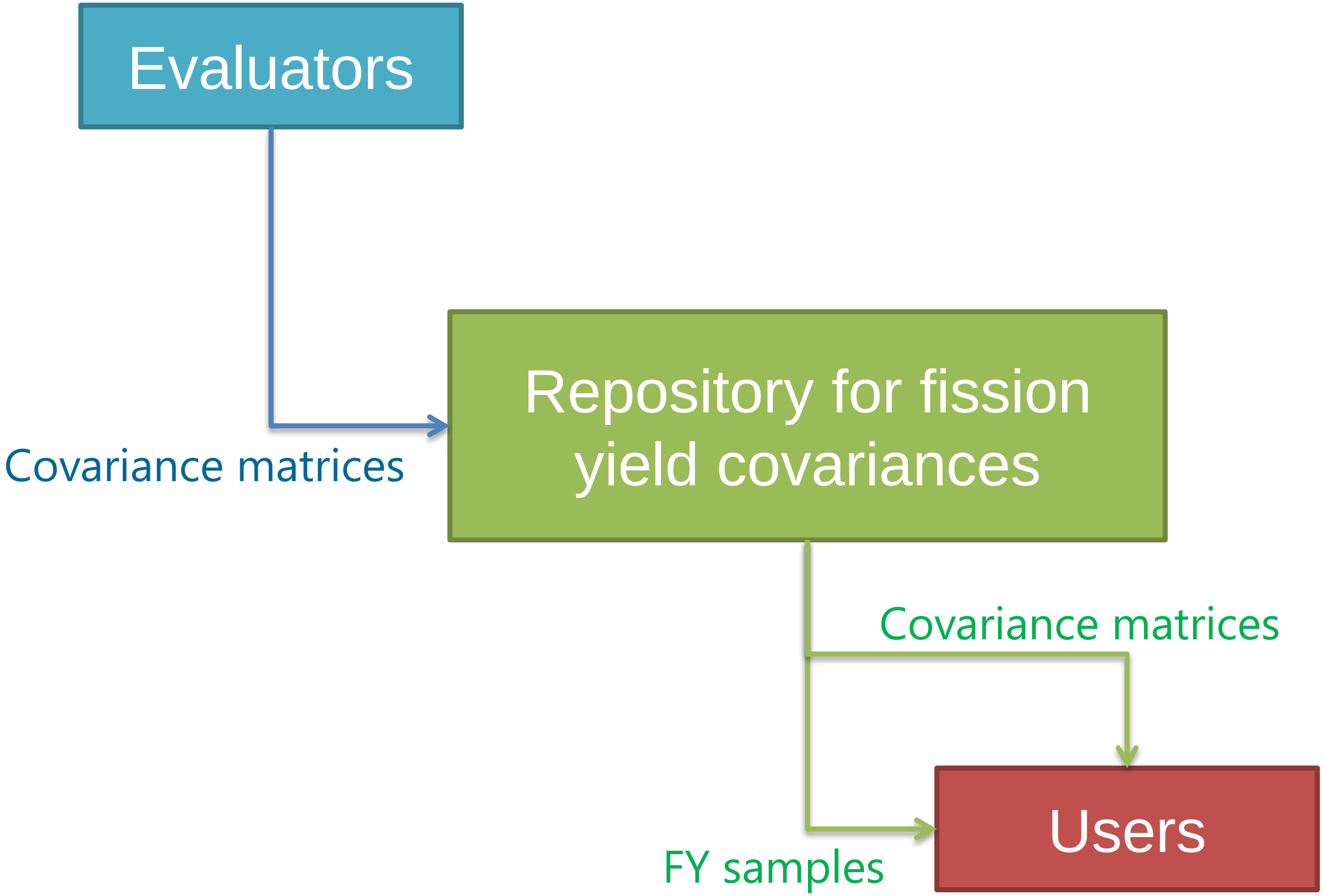
Documentation

- JEFF Reports
- JEF Docs
- Fusion Docs
- References

Next Meetings

24-27 April 2017

NEA proposed actions


Evaluators

Covariance matrices

Repository for fission yield covariances

Covariance matrices

FY samples

Users

Any questions?