

Progress of the WPEC sub-group 37

Dr Robert W. Mills,
NNL Research Fellow for Nuclear Data,
UK National Nuclear Laboratory.

- Task 1: Document and compare existing methodologies.
 - Description of current and proposed JEFF fission product yield evaluation methodologies- R Mills
- Task 2: Insights, new measurements to understand and reconcile discrepancies.
 - Covariance Matrix Evaluation for Independent Fission Yields- N Terranova
 - Merging GEF into TALYS – S. Pomp
 - Recent work on the GEF code – (K-H Schmidt)
- Task 3: Possible new fission product data, format and covariance data.
 - Status on fission yield perturbation methodology at PSI using CASMO-5- O. Leray
 - Impact of the fission yield covariance data in burn-up calculations– (O. Cabellos)

- The subgroup was approved to:

R. Mills, on behalf of the JEFF project, proposed a new subgroup with the objective to improve fission product yield evaluation methodology. The goal is for the experts in this field to develop improved methodologies for future evaluations that are consistent with the new theoretical knowledge and experimental measurements, and include common covariance methods that will allow calculations with both improved accuracy and the generation of uncertainties on calculated engineering parameters. This proposal is supported by the ENDF project and M. Chadwick accepted the role of subgroup monitor. *The proposed subgroup would start in January 2013. The WPEC approved the proposal and established the subgroup as number 37.*

- JEFF-3.2 (December 2014)
 - Adopt GEF to replace models
 - Need to extend model to low yields and “merge” with experimental data.
 - >1000 new measurements (mostly Lohengrin)
 - Otherwise same systems and “average spectra”
- JEFF-3.3 (2016/17)
 - Adopt GEF results for thermal to 20 MeV
 - >100 spontaneous and neutron fissioning systems
 - Covariance matrices (method to be determined)
 - Adjust to experimental data (MATCH code)?

Covariance Matrix Evaluation for Independent Fission Yields

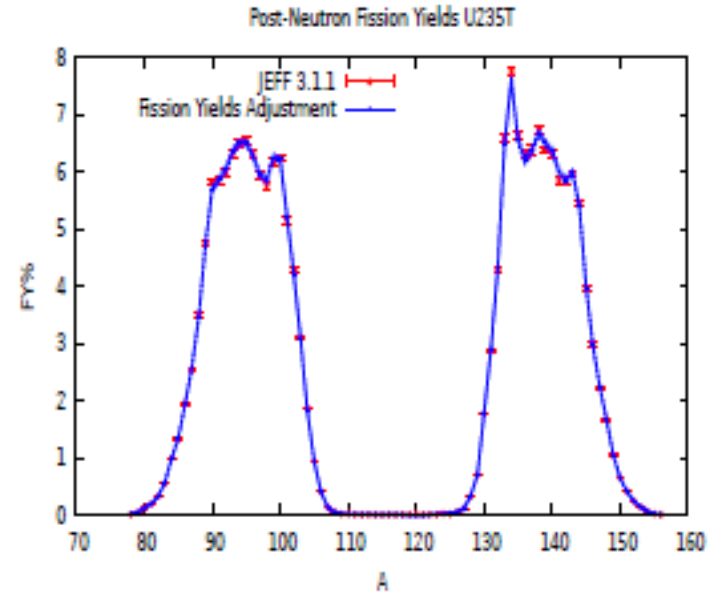
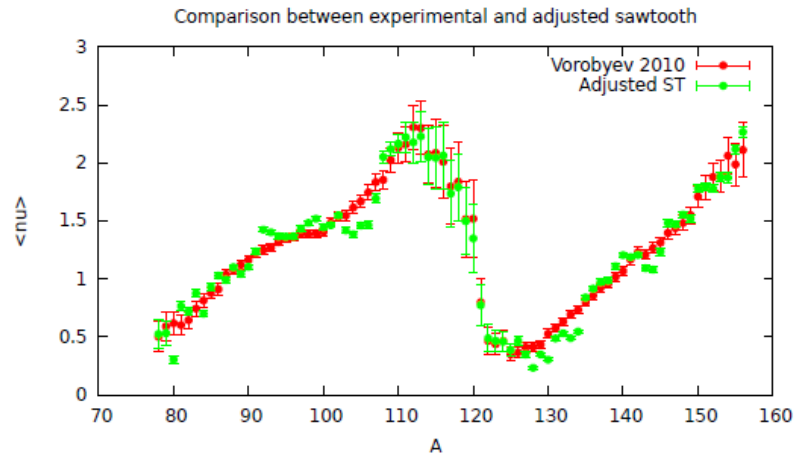
N. Terranova¹, O. Serot², P. Archier², C. De Saint Jean², M. Sumini¹

¹Dipartimento di Ingegneria Industriale (DIN), Università di Bologna, Italy

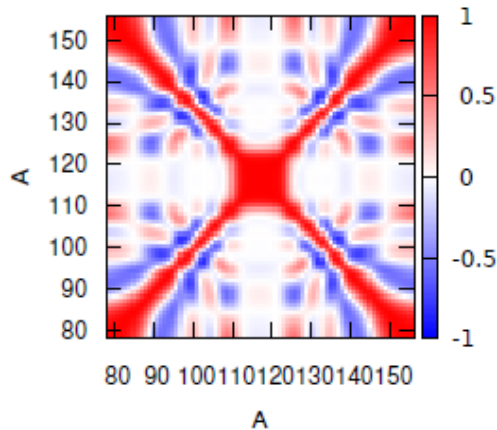
²CEA, DEN, Cadarache, F-13108 Saint Paul les Durance, France

- They have developed a method able to represent faithfully JEFF 3.1.1 evaluations for mass fission yields in the CONRAD system.
- The adjustment of the parameters for the pre-neutron fission modes and the saw-tooth curve has given acceptable results.
- Preliminary correlation information have been produced for mass fission yields, considering only statistical uncertainties.
- For future to consider systematic uncertainties, charge and isomeric yields

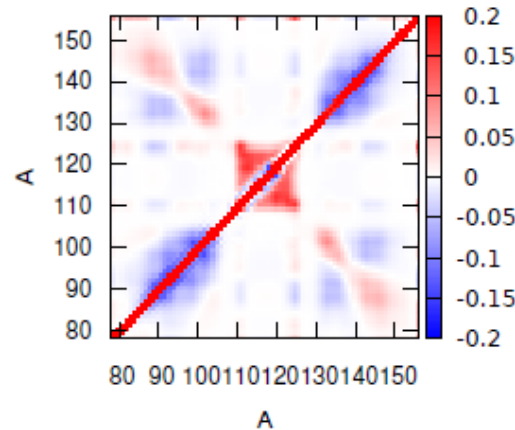
Covariance Matrix Evaluation for Independent Fission Yields



Only fission mode parameters propagated



All parameters propagated



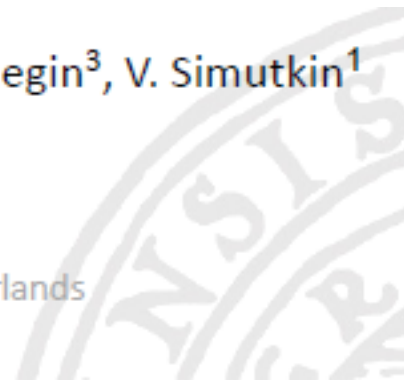
Fission yield calculations with TALYS/GEF

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¹ Uppsala University, Div. of applied nuclear physics, Sweden

² Nuclear Research and Consultancy Group, Petten, The Netherlands

³ PNPI, Gatchina, St. Petersburg, Russia

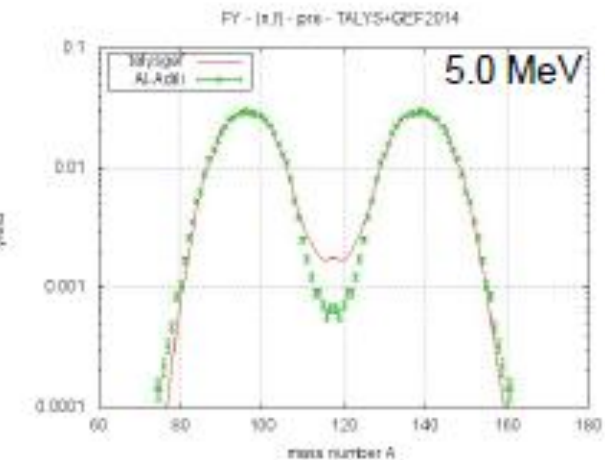
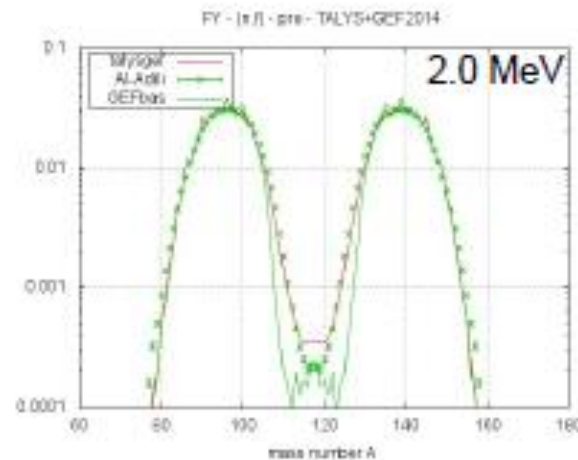
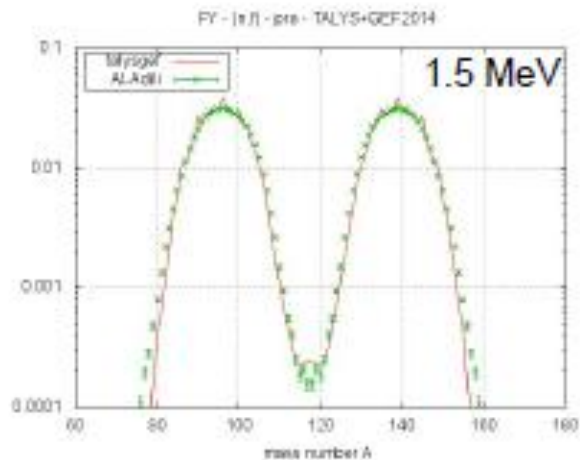
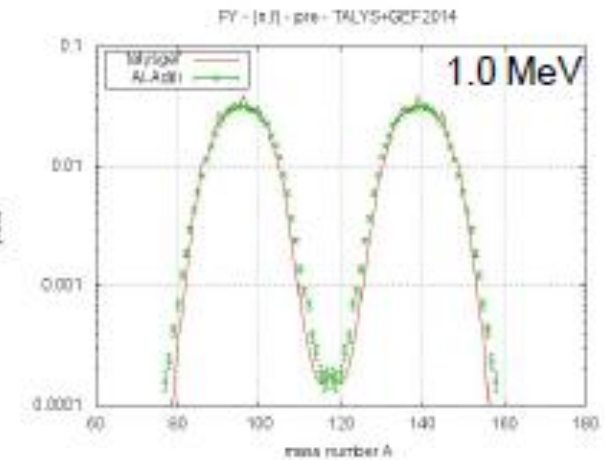
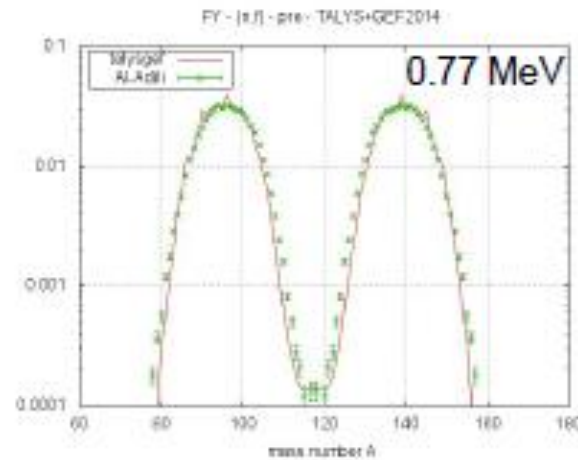
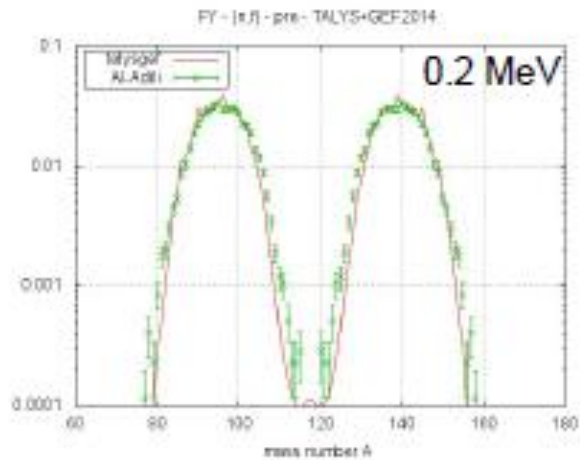


Motivation

- Complement TALYS (state-of-the-art, comprehensive nuclear reaction modelling code) for TMC and TENDL
 - Option to replace TANES and TAFIS in the T6 code package with GEF
 - Produce complete and consistent ENDF
- Add TALYS capabilities to GEF: handling of pre-fission stages and de-excitation

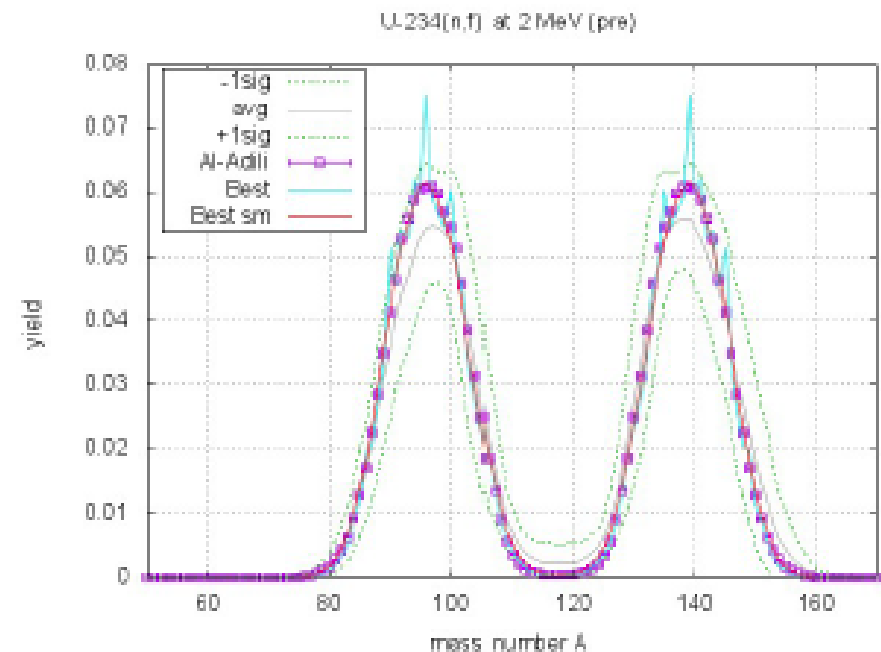
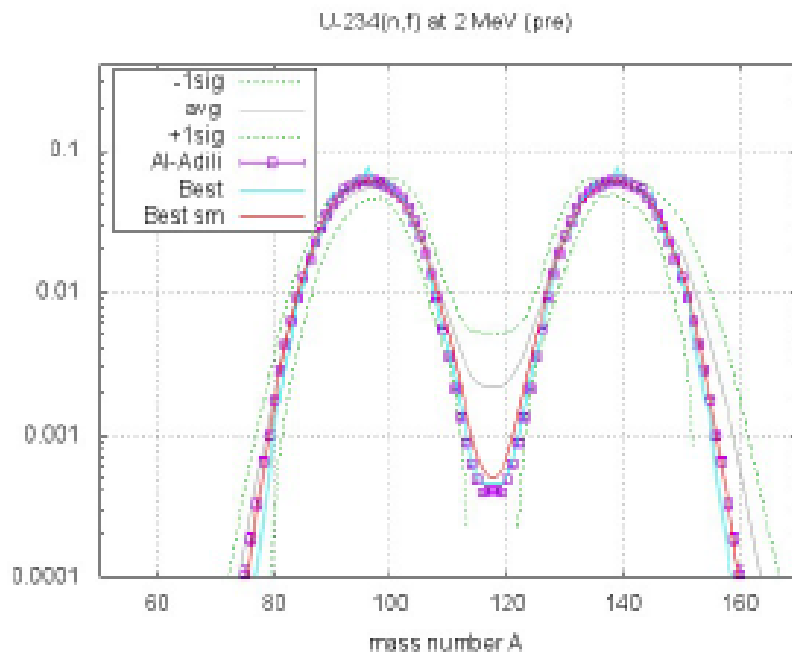
Fission yield calculations with TALYS/GEF

Compare results with U234(n,f) from PhD thesis Al-Adilli (2013)



Fission yield calculations with TALYS/GEF

500 TALYS+GEFSUB runs with randomization of 18 GEF parameters
(10 times the uncertainties as given in GEF report from April 2014)



red curve: best TALYS+GEF run; adjusted to exp. resolution (4.5 AMU)

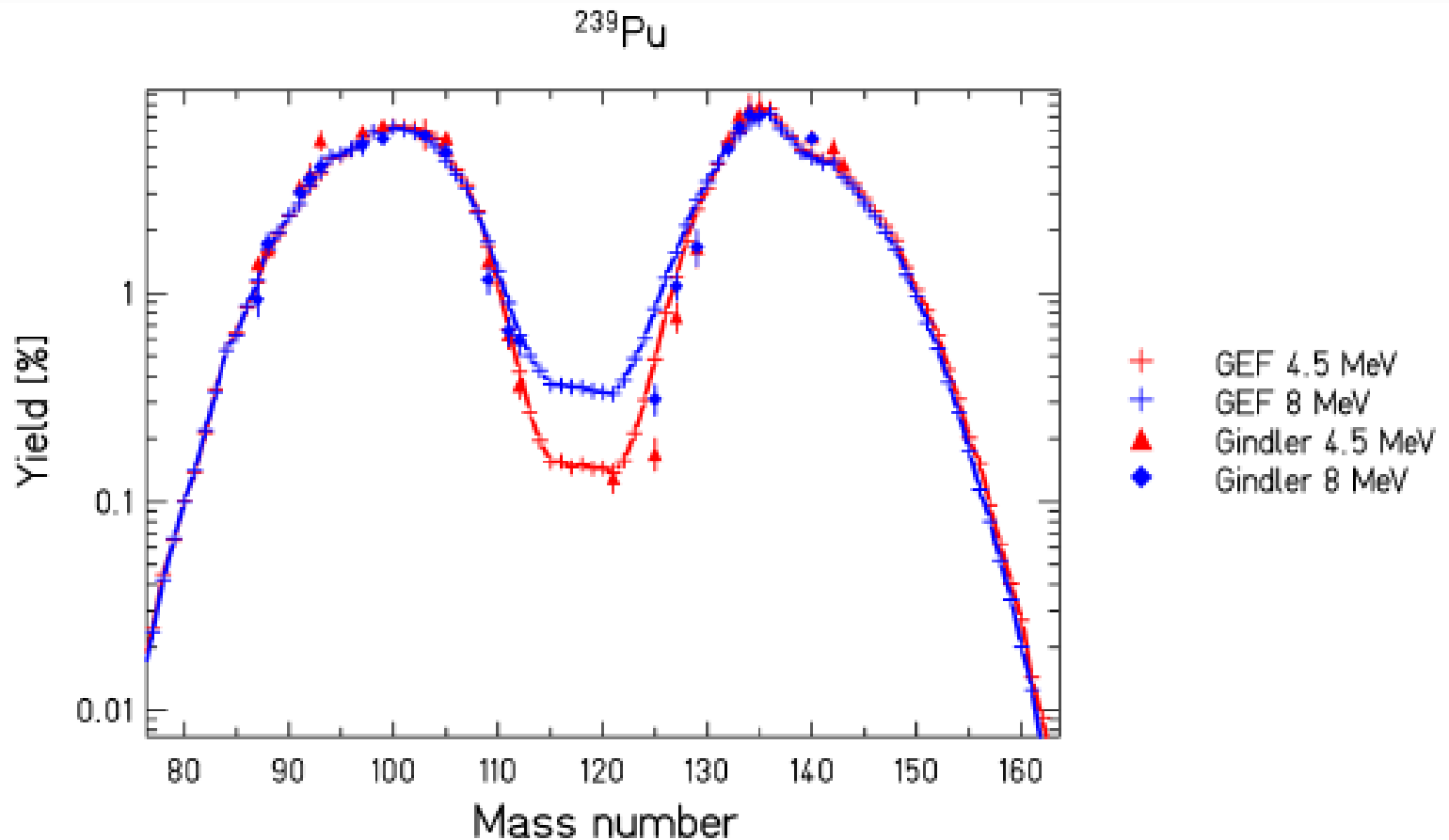
Under construction for next TALYS



- Karl-Heinz Schmidt provides FORTRAN subroutine GEFSUB
- GEFSUB returns (Z_f , A_f , E_x , J) arrays, i.e. for **each** fission fragment the J -dependent excitation energy grid, **before** neutron emission.
- At the end of a “conventional” TALYS calculation, i.e. when the nuclear structure arrays for the actinides can be flushed, a loop over all fission fragments is performed, still inside the same TALYS run, to deplete all excitation energy grids of these fission fragments. This gives:
 - Post-neutron FY for each Z,A
 - ν as function of number of neutrons, $P(\nu)$, fission product, $\nu(Z,A)$, and average number of prompt fission neutrons, $\bar{\nu}$.
 - The same for gamma's (and charged particles for high energies)
 - PFNS and PFGS, etc.
 -but this time calculated with the full Hauser-Feshbach and pre-equilibrium models of TALYS, including all flexibility for adjustment. Optimization and covariances.
- Already present in TALYS: JEFF-3.1.1 Radioactive Decay Data File:
 - Independent and cumulative yields
 - Feeding of any isomer, including beta delayed precursors

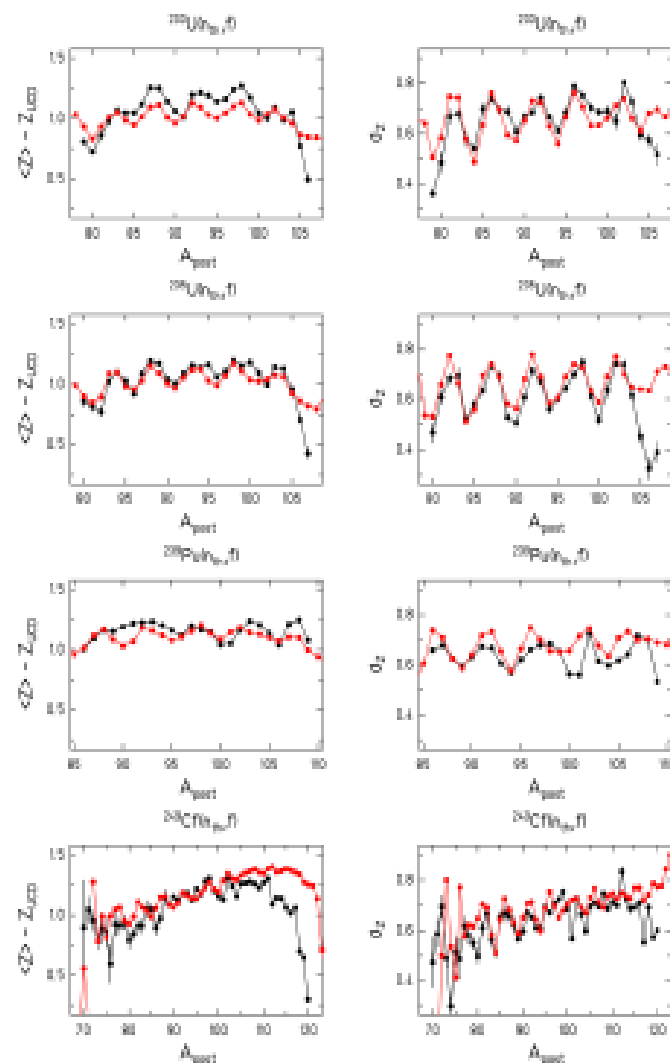
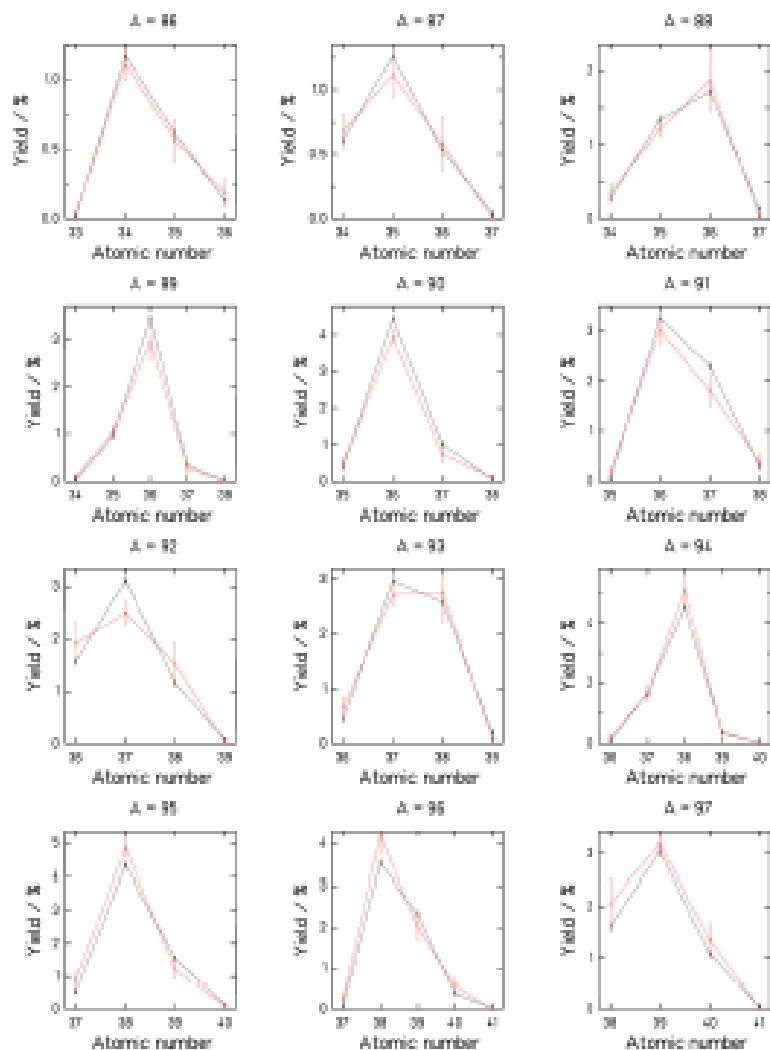
- Summary of 4 recent JEF/DOC from the recent JEFF presented on behalf of K-H Schmidt.
- For more details see 200 page GEF report.
- Model based upon ~50 parameters for all fission systems
- now includes multi-chance fission, isomeric yields
- Can calculate covariance matrices, which can be coupled with MATCH code to adjust data and develop covariance matrices.

FF mass distributions (4, 8 MeV)



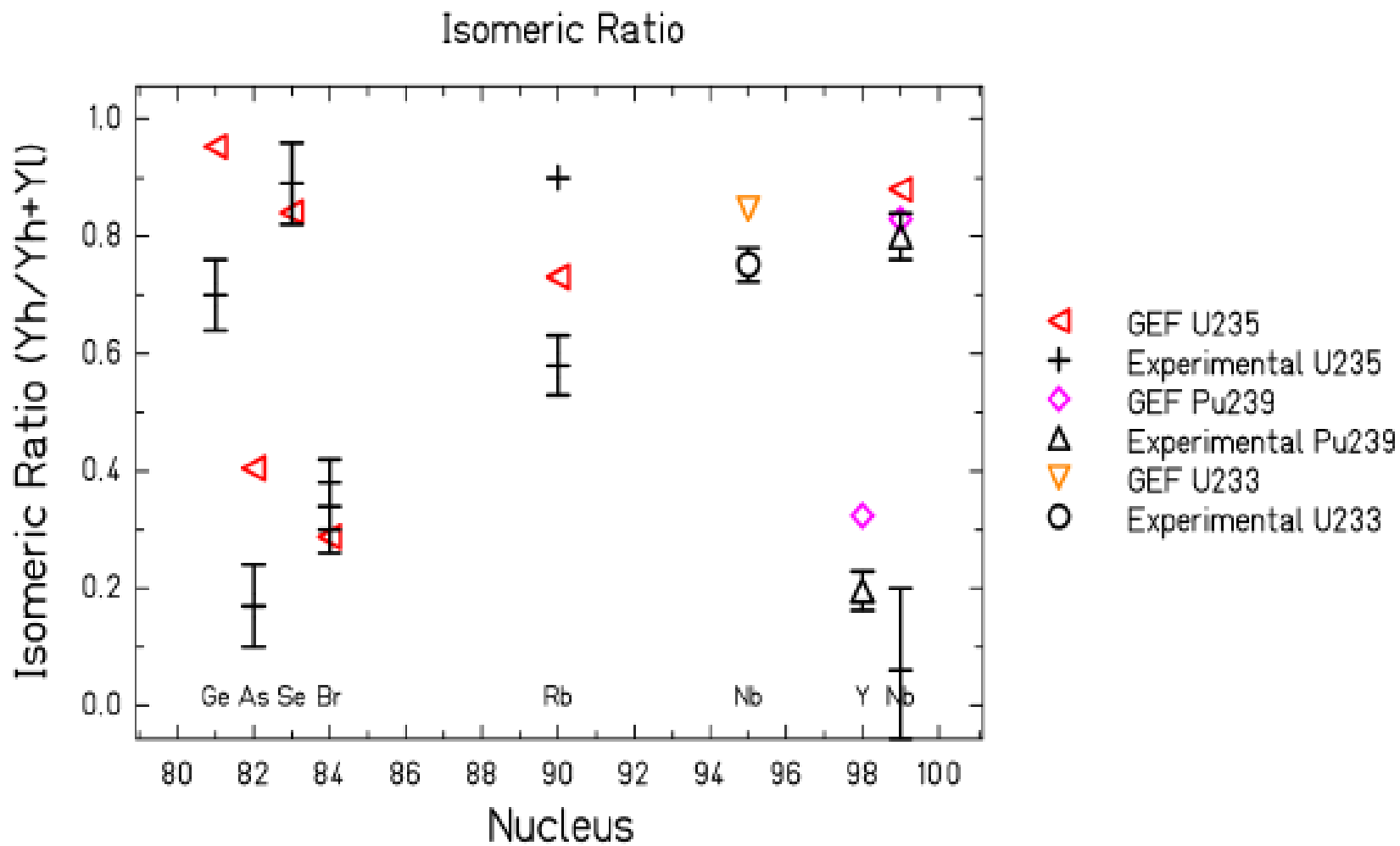
Data are scarce at intermediate energies.

FF nuclide distributions

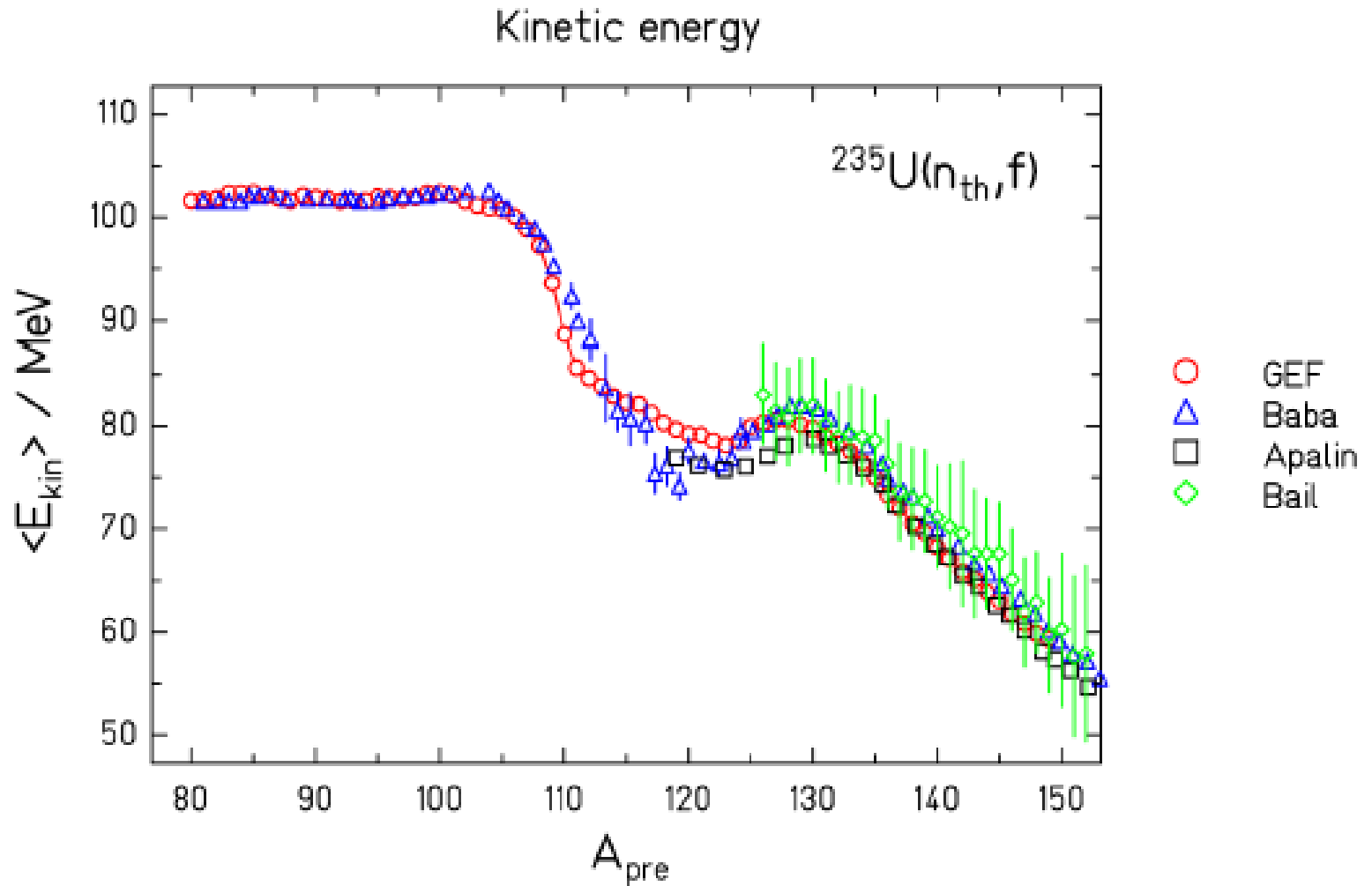


$^{235}\text{U}(nth, f)$

Isomeric yields

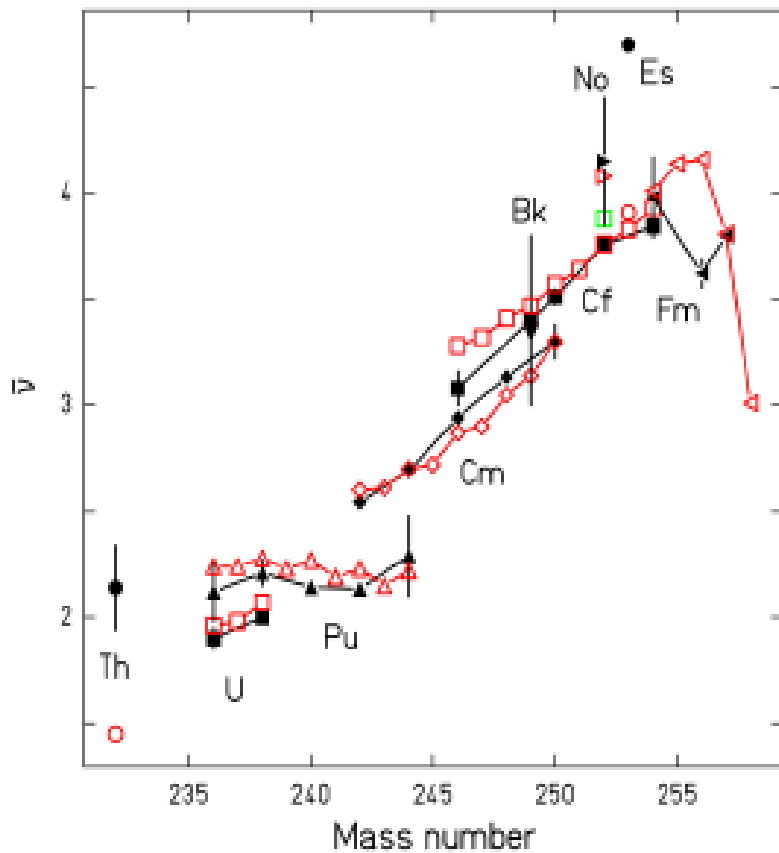


FF kinetic energies



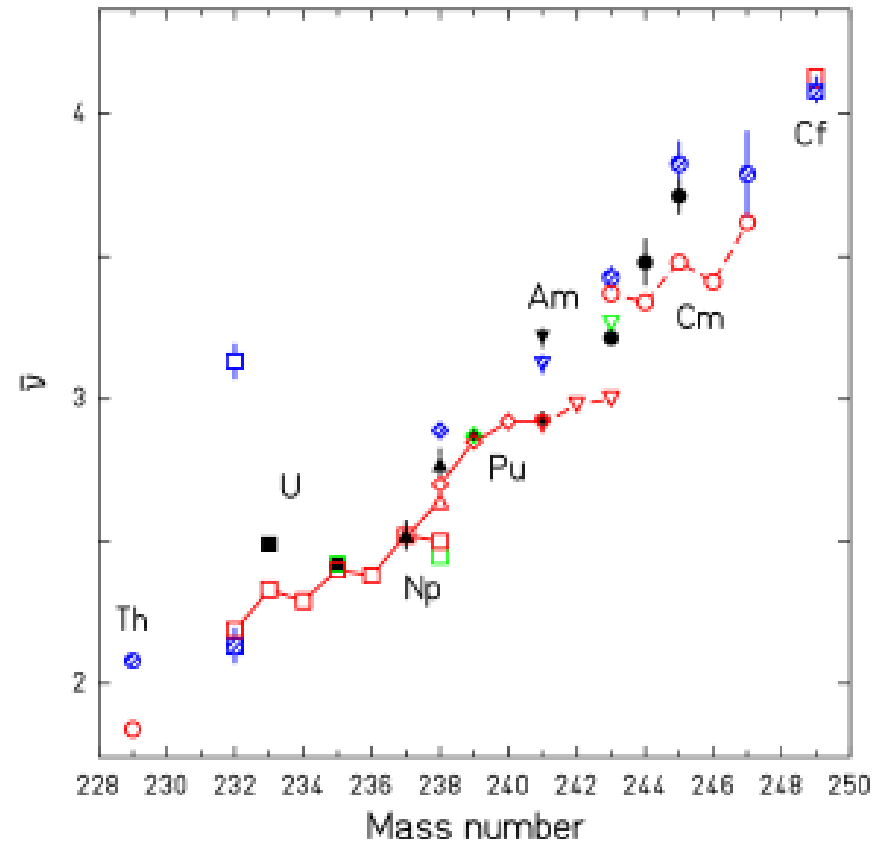
nu-bar

Prompt-neutron yields for spontaneous fission

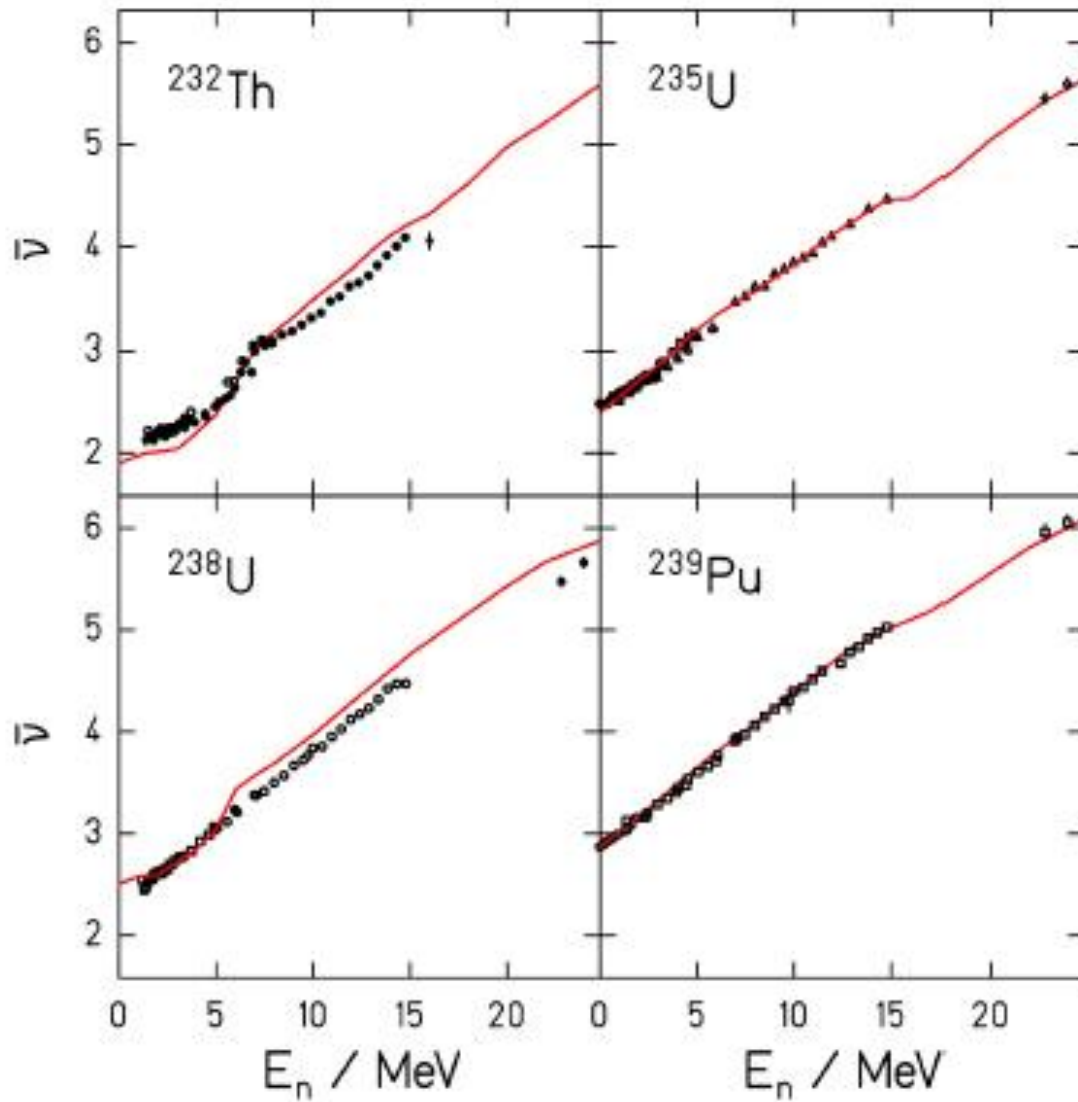


rms deviation: 0.1 units

Prompt-neutron yields for (n_{th}, f)

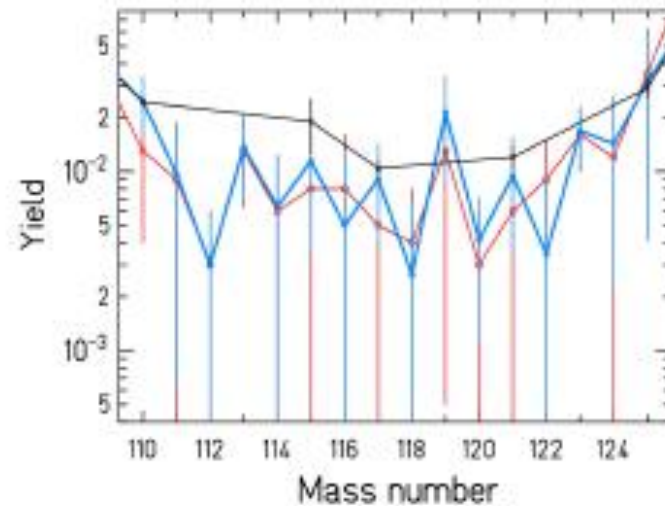
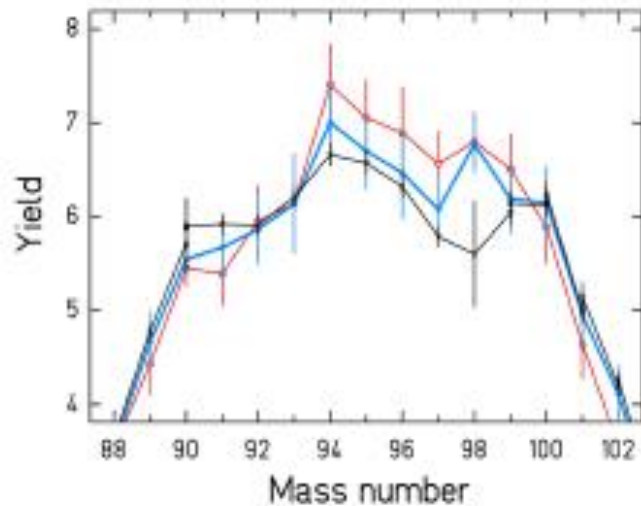
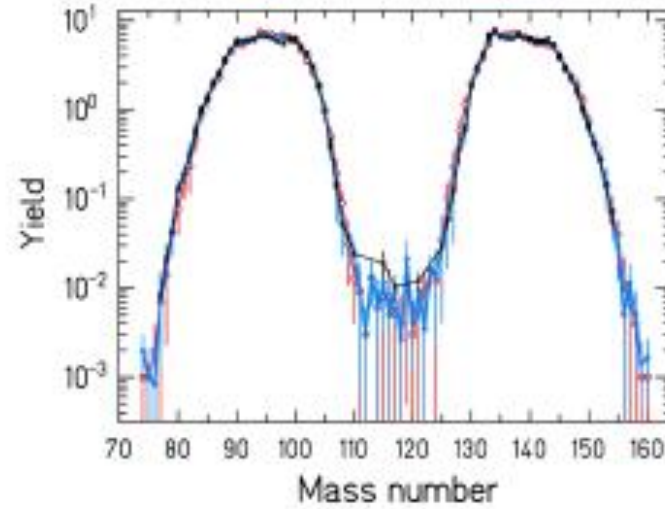
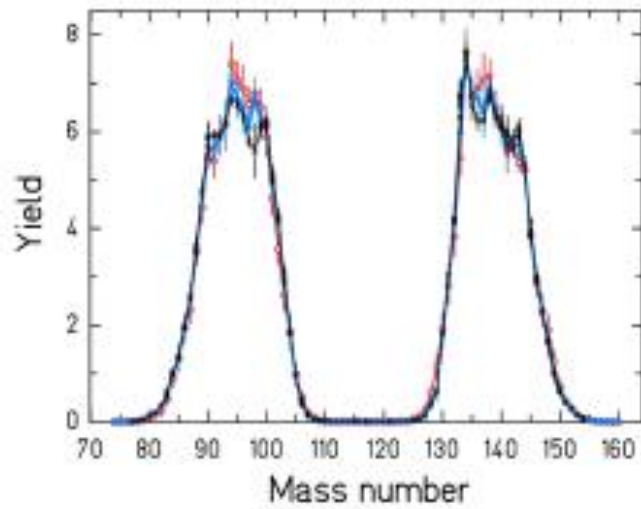


nu-bar (E)



Example 1

U235T

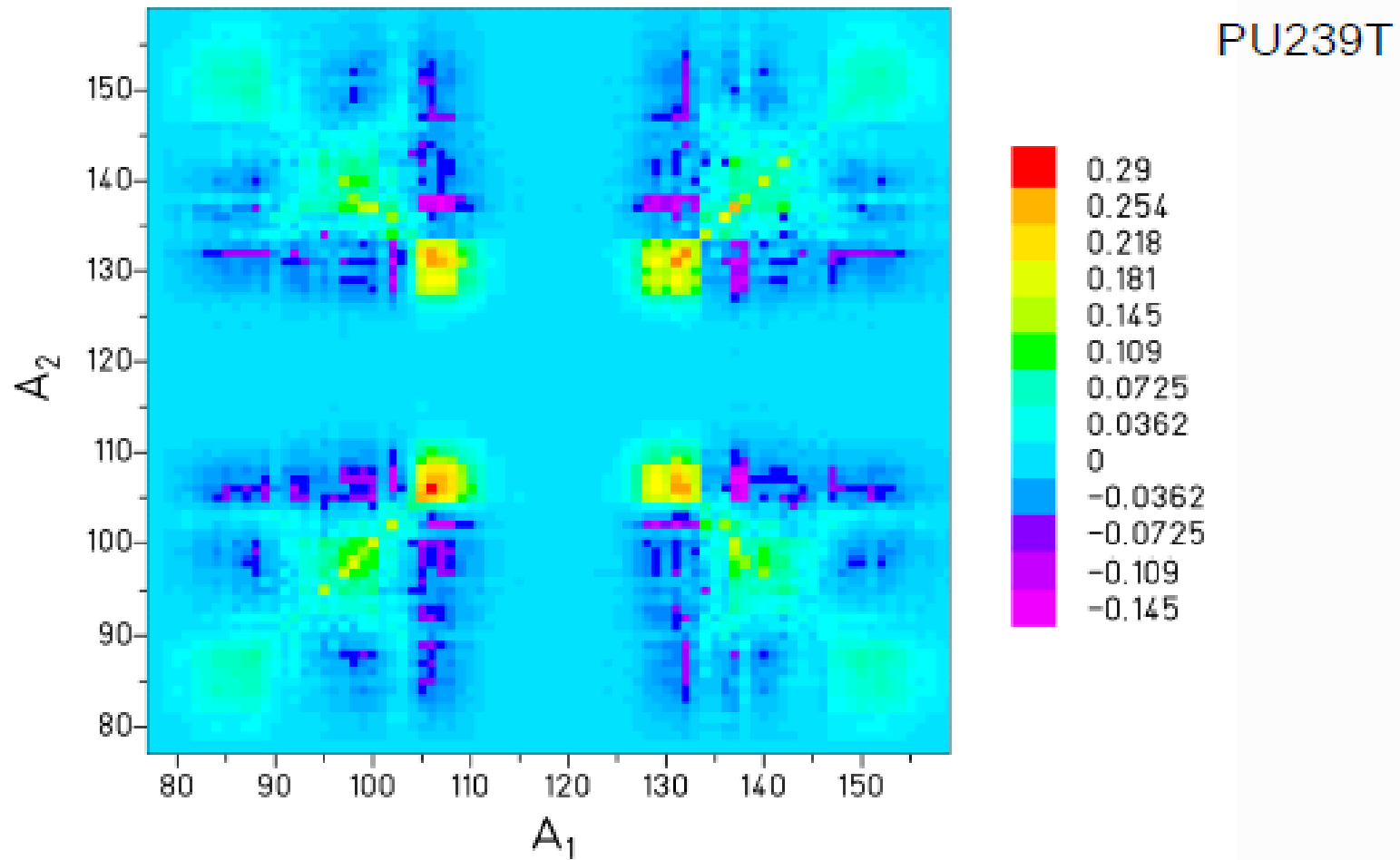


Data

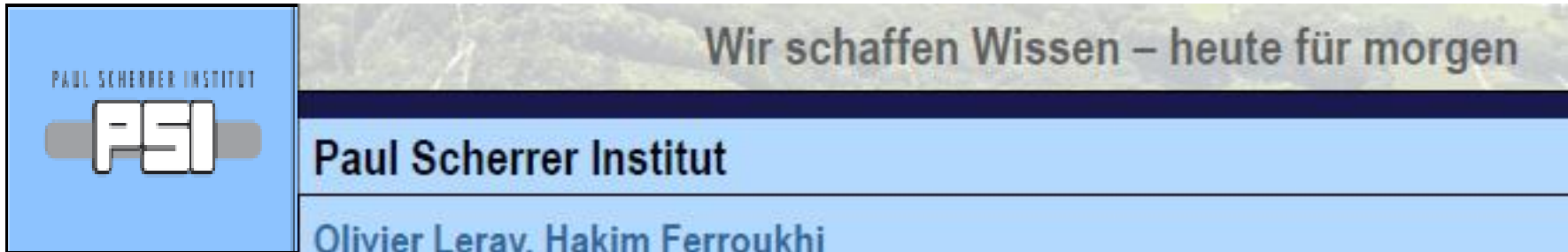
GEF

MATCH

Full covariance matrix



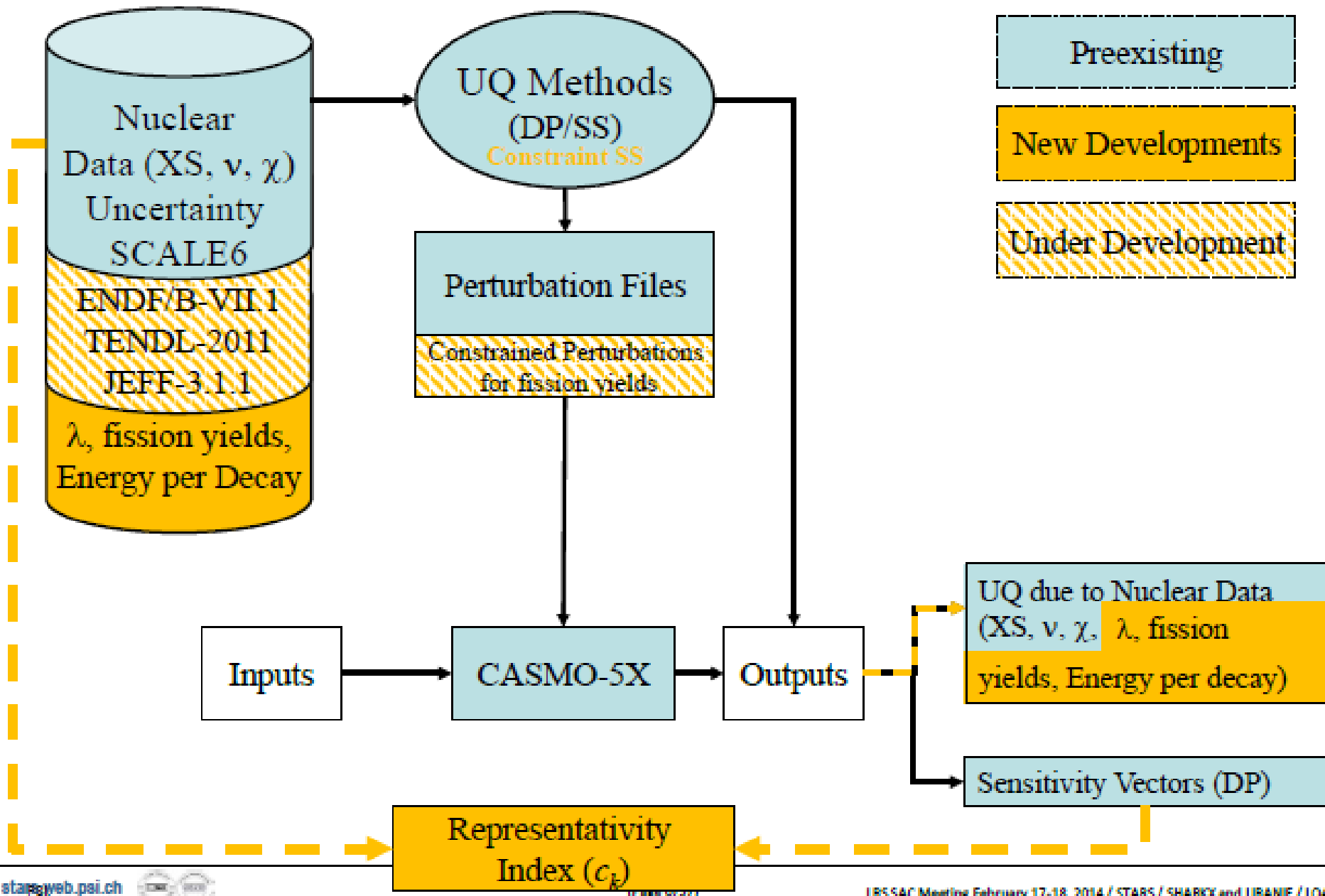
Determined by the inner logic of the model.
Basically different from experimental covariances!



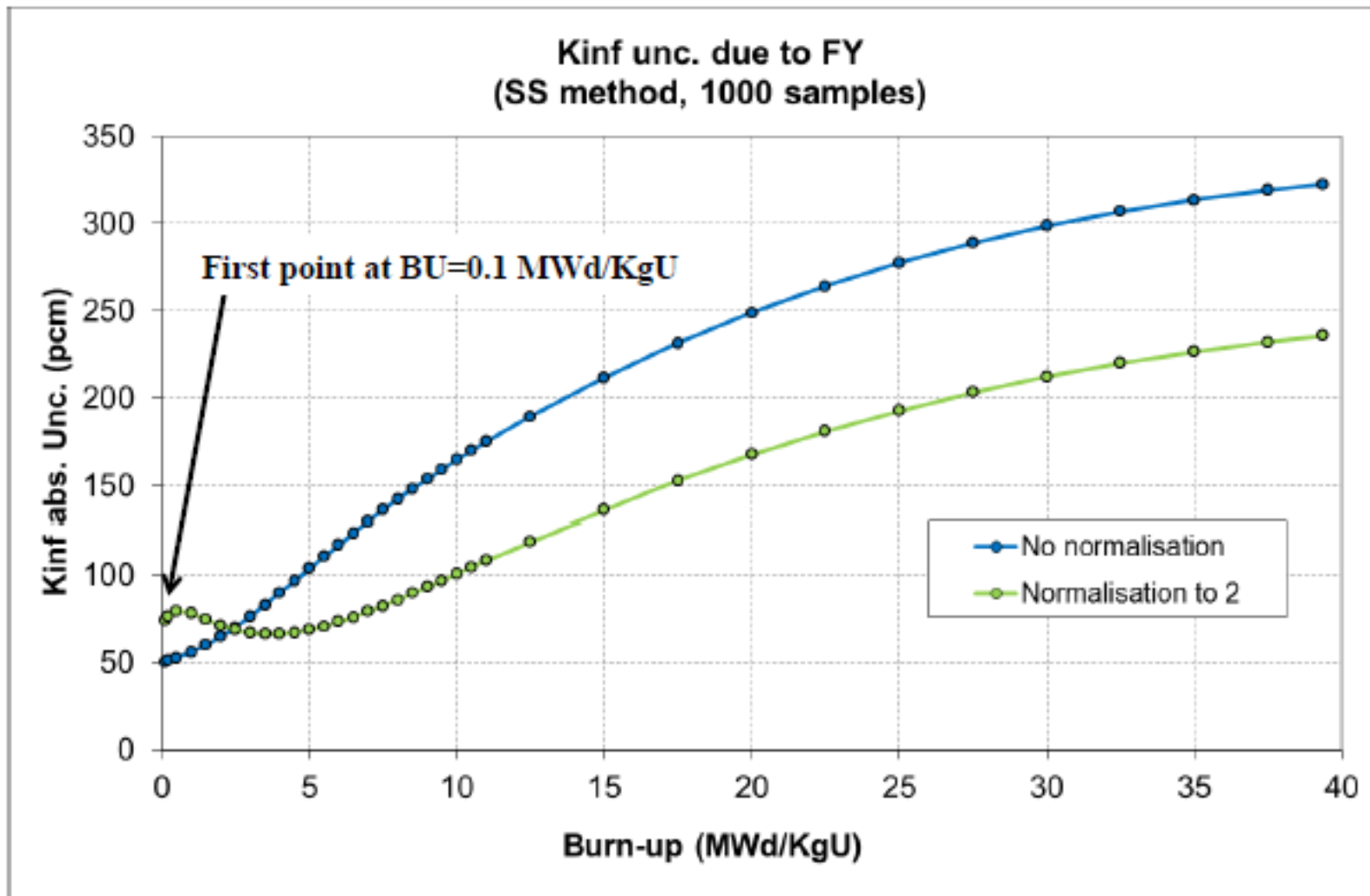
- Recent developments of the SHARK-X tool using
 - Direct perturbation (brute force) and Statistical Sampling
 - Adjustment of FY data in CASMO to force physical constraints
 - Considers problems with PDF (-ve parameters)
- Motivation is to calculate uncertainties on decay heat, isotopic composition and reactivity.

2. THE SHARK-X TOOL

Recent Development in SHARK-X



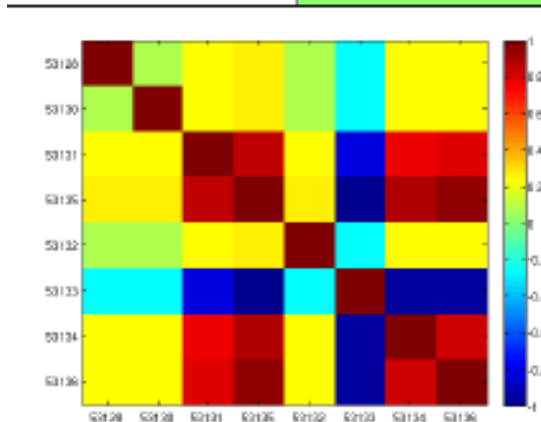
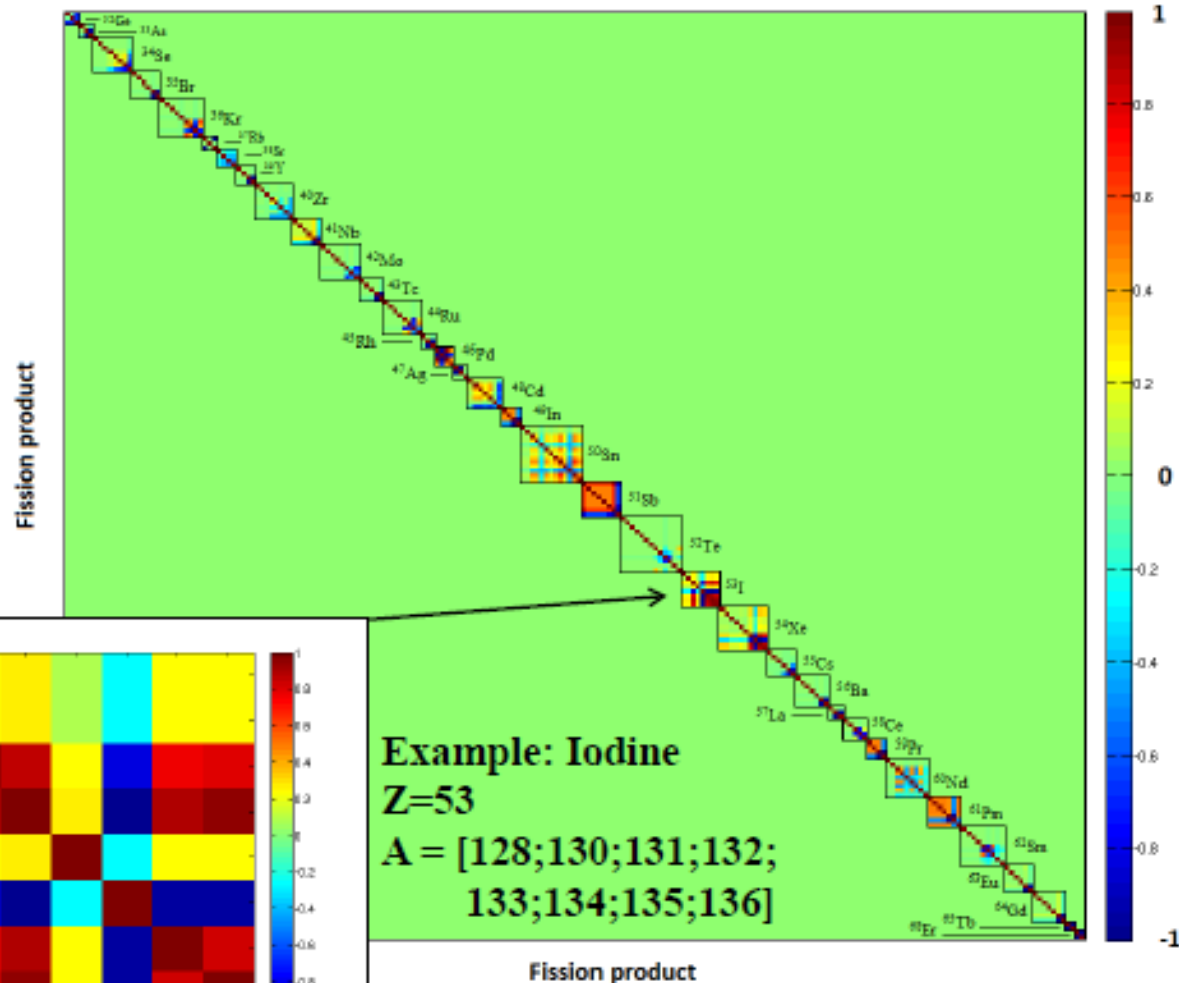
Status on fission yield perturbation methodology at PSI using CASMO-5



UAM Phase II Benchmark (case2a: PWR UO₂ Fuel Assembly)

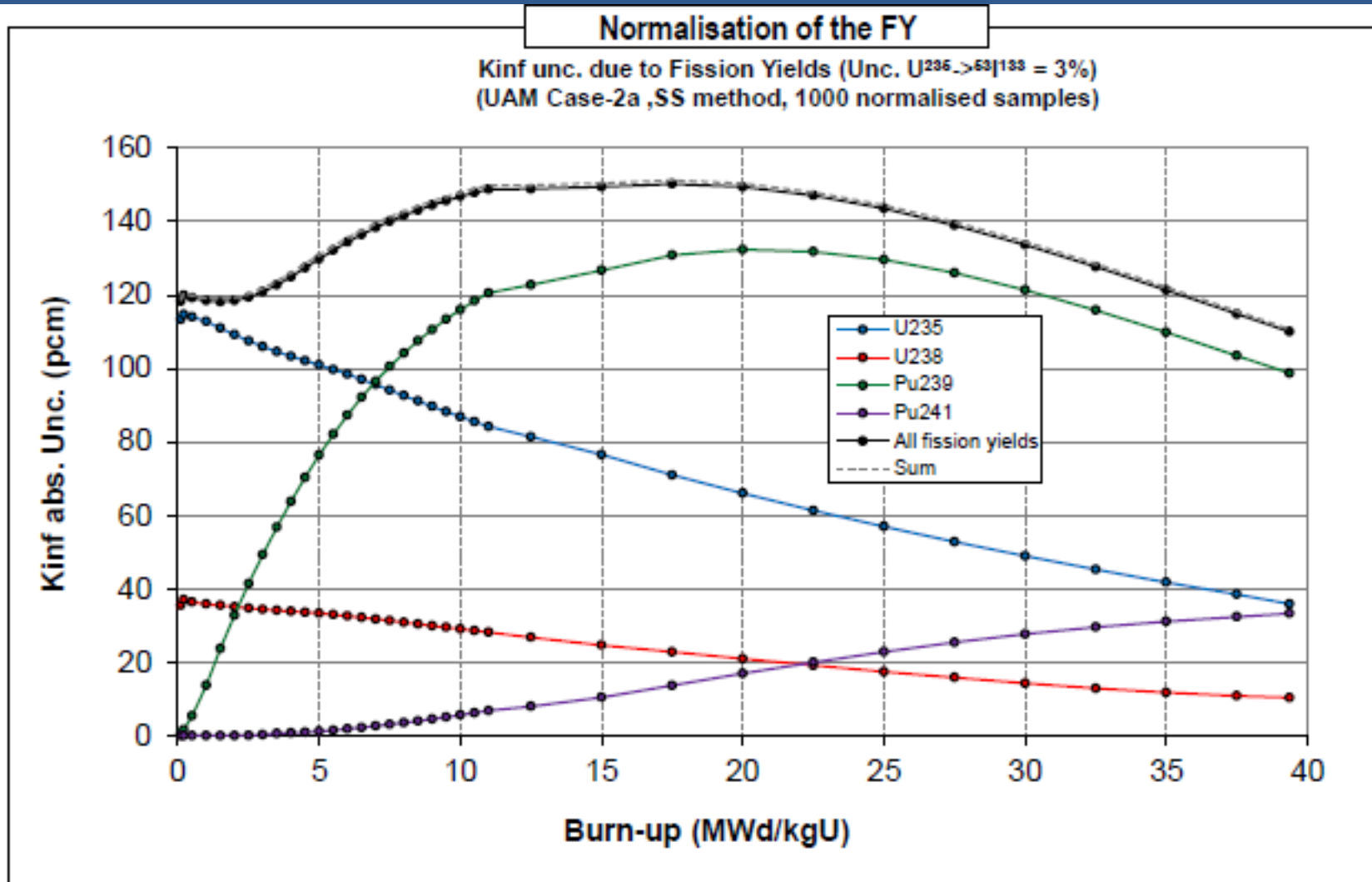
Status on fission yield perturbation methodology at PSI using CASMO-5

Fission Yield Correlation matrix for U^{235} (215 daughters, 35 elements) Correlation:



Example: Iodine
Z=53
A = [128;130;131;132;
133;134;135;136]

Status on fission yield perturbation methodology at PSI using CASMO-5



IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS



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- Burnup Credit “Pin-cell Burn-up UAM Benchmark”
 - Propagation of FY Uncertainties in “pin-cell burn-up Benchmark”
- Methodology to propagate ND Uncertainties on number densities
 - Monte Carlo and S/U Methodologies
- Uncertainty Propagation: “Criticality Uncertainty”

IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

➤ References on FY uncertainty calculations:


- ❑ J.S. Martínez et al., "GRS Results for the Burnup Pin-cell Benchmark Propagation of Cross-Section, Fission Yields and Decay Data Uncertainties", 7th Int. Workshop on Uncertainty Analysis in Modeling, OECD/NEA, Paris, France. 10-12 April 2013.

- Implemented in XSUSA Methodology (Monte Carlo) using FY-ENDF/B-VII.1

		0 GWd/MTU		10 GWd/MTU			30 GWd/MTU			60 GWd/MTU				
		mean	mean	rel. std. dev.			rel. std. dev.			rel. std. dev.				
				ΔXS	ΔDD	ΔFYs	ΔXS	ΔDD	ΔFYs	ΔXS	ΔDD	ΔFYs		
Nd-148	GRS	0.00E+00	1.76E-06	0.3	0.0	16.5	5.58E-06	0.3	0.0	14.5	1.18E-05	0.4	0.0	13

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Fission yield covariance generation and uncertainty propagation through fission pulse decay heat calculation

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FY covariance data generation:

- Great efforts have been committed to develop methodologies for correlation generation (full covariance matrices) for FY data.
- This task is in the scope of the framework of WPEC-SG37.

Methodologies proposed at the kick-off meeting of WPEC-SG37 (May 2013), based on:

- Perturbation theory applied to the “Five Gaussians and Wahl’s models” (*Musgrove et al., 1973; Wahl, 1988*), proposed by *Pigni et al. (2013)*.
- Monte Carlo parameter perturbation using the GEF code (*Schmidt and Jurado, 2010*), presented by Schmidt (*2013*).
- Bayesian/general least-squares (GLS) method, where the IFY covariance matrix is updated with information on the chain yields as proposed by *Kawano and Chadwick (2013)*, and previously applied by *Katakura (2012)*.
 - A variation of this proposal, with IFYs covariance matrix updated with CFYs ones is described and reported by UPM/SCK (*L. Fiorito et al., 2014*)

IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

The updating process is represented by Eqs.

(11) and (12),

$$\theta - \theta_0 = V_0 S^t (S V_0 S^t + V)^{-1} (\eta - y_0) \quad (11)$$

$$V_s = V_0 - V_0 S^t (S V_0 S^t + V)^{-1} S V_0 \quad (12)$$

where V_0 is the variance matrix of prior estimates of the parameters (θ_0), V is the variance matrix of the introduced data fitting the constraining system (η), and V_s is the updated covariance matrix of the system parameters (θ). Superscript t refers to the transpose of a matrix.

Simple equations to generate the updated covariance matrix for IFYs can be derived from Eq. (12), resulting in Eqs. (13) and (14) which represent the diagonal and off-diagonal terms respectively:

$$\mu_{ii} = \sigma_i^2 \left(1 - \frac{\sigma_i^2}{\sigma^2 + \sum_j \sigma_j^2} \right) \quad (13)$$

$$\mu_{ij} = - \frac{\sigma_i^2 \sigma_j^2}{\sigma^2 + \sum_j \sigma_j^2} \quad (14)$$

Here, σ_i is the standard deviation of the i th IFY and σ is the standard deviation of evaluated MFY. Sum $\sum_j \sigma_j^2$ includes all the isotopes in the same mass chain as it relates MFYs to IFYs.

Ref. : "Fission Yield Covariance generation ...", L. Fiorito et al. Annals of Nuclear Energy, 2014

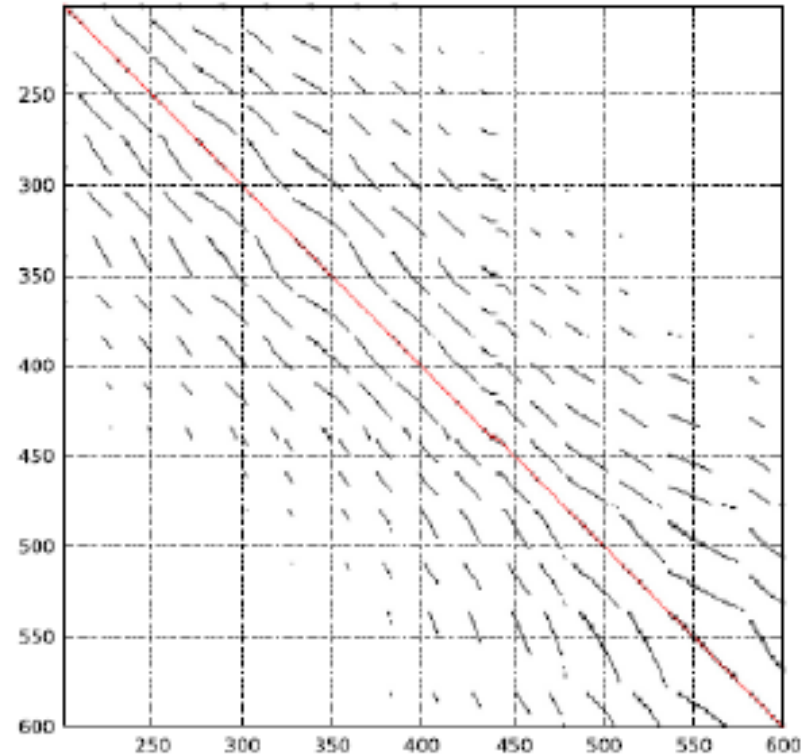


Fig. 2. Section of the IFY correlation matrix of ^{235}U thermal fission for ENDF/B-VII.1 obtained by updating with MFY uncertainties. Red dots are positive correlations and black dots are negative correlations, otherwise no correlation exists. Each matrix index refers to one FP of the studied fissionable system, once the FPs are sorted by ZZZAAAM (Z, charge; A, mass; M, isomeric state) in increasing order (e.g. index 1 refers to the lowest ZZZAAAM value). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

□ Monte Carlo burnup calculation SCALE6.1.2/TRITON

- Generation of a set of 1000 FY random libraries for U^{235} and Pu^{239}

"No-correlation". FY uncertainty is the standard deviation of ENDF/B-VII.1	"Correlation" matrix using Katakura methodology
$V_D = \begin{bmatrix} \left(\frac{\Delta Y_1}{Y_1}\right)^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \left(\frac{\Delta Y_K}{Y_K}\right)^2 \end{bmatrix}$	$V_D = \begin{bmatrix} \left(\frac{\Delta Y_1}{Y_1}\right)^2 & \left(\frac{\text{cov}(Y_1, Y_2)}{Y_1 Y_2}\right) \dots & \left(\frac{\text{cov}(Y_1, Y_K)}{Y_1 Y_K}\right) \\ \vdots & \ddots & \vdots \\ \left(\frac{\text{cov}(Y_K, Y_1)}{Y_K Y_1}\right) & \dots & \left(\frac{\Delta Y_K}{Y_K}\right)^2 \end{bmatrix}$

- PDF: Normal distribution, with "zero" for negative values.

□ Sensitivity/Uncertainty calculation SCALE6.1.2/TRITON

- Calculation of Sensitivity coefficients: $S_{FY_{ij}}^U = (\Delta N_i / N_i) / (\Delta FY_{ij}^U / FY_{ij}^U)$
- S/U: 1st Order Approximation, "Sandwich Formula"

$$\frac{\text{var}(N_i)}{N_i^2} = (S_{FY_{i1}}^{U^{235}} \quad S_{FY_{i1}}^{Pu^{239}} \quad \dots) \begin{bmatrix} V_{U^{235}} & 0 & 0 \\ 0 & V_{Pu^{239}} & 0 \\ 0 & 0 & \ddots \end{bmatrix} \begin{pmatrix} S_{FY_{i1}}^{U^{235}} \\ S_{FY_{i1}}^{Pu^{239}} \\ \vdots \end{pmatrix}$$

IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

Table 3. Uncertainty in number density (in %) for some important fission products at 60 GWd/MTU. Fission Yield source of uncertainty (standard deviation) is taken from ENDF/B-VII.1.

Nuclide	GRS			Nuclide	GRS		
	Corr.	No corr.	XSUSA		Corr.	No corr.	XSUSA
⁷⁹ Se	3.5	16.0	-	¹⁴² Nd	0.8	3.5	-
⁹⁰ Sr	0.8	6.2	-	¹⁴³ Nd	0.4	6.5	5.9
⁹⁵ Mo	0.5	8.4	7.9	¹⁴⁴ Nd	0.2	3.9	-
⁹⁹ Tc	0.8	10.0	9.5	¹⁴⁵ Nd	0.4	7.1	6.7
¹⁰¹ Ru	0.7	4.6	-	¹⁴⁶ Nd	0.7	10.8	-
¹⁰⁶ Ru	1.2	13.7	-	¹⁴⁸ Nd	0.8	13.7	13.0
¹⁰³ Rh	1.1	12.1	-	¹⁴⁷ Pm	0.6	10.3	-
¹⁰⁹ Ag	10.9	17.8	-	¹⁴⁷ Sm	0.5	9.4	-
¹²⁵ Sb	4.2	19.1	-	¹⁴⁹ Sm	0.6	12.2	10.6
¹²⁹ I	2.7	20.7	-	¹⁵⁰ Sm	0.6	10.3	-
¹³⁵ I	2.8	4.3	-	¹⁵¹ Sm	0.7	11.7	-
¹³¹ Xe	0.4	6.9	-	¹⁵² Sm	0.6	11.3	8.8
¹³⁵ Xe	0.4	5.1	-	¹⁵¹ Eu	0.7	12.1	-
¹³³ Cs	0.3	3.4	1.7	¹⁵³ Eu	0.8	9.9	-
¹³⁴ Cs	0.3	3.0	-	¹⁵⁴ Eu	0.8	10.4	-
¹³⁵ Cs	0.3	3.4	-	¹⁵⁵ Eu	1.0	9.5	-
¹³⁷ Cs	0.5	1.5	1.7	¹⁵⁵ Gd	1.0	10.5	8.8
¹³⁹ La	0.9	3.2	-	¹⁵⁶ Gd	1.2	9.0	-
¹⁴⁴ Ce	0.2	8.0	-	¹⁵⁷ Gd	1.3	9.5	-
				¹⁵⁸ Gd	2.3	11.3	-

- i) No correlation between fission products (Δ FYs/No corr.)
- ii) FYs including correlations for ²³⁵U and ²³⁹Pu taken from Katakura methodology (Δ FYs/Corr.)
- iii) GRS calculation

IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

S/U, Applying “Sandwich Formula”:

$$\frac{\text{var}(N_i)}{N_i^2} = (S_{FYI}^{U235} \quad S_{FYI}^{Pu239} \quad \dots) \begin{bmatrix} V_{U235} & 0 & 0 \\ 0 & V_{Pu239} & 0 \\ 0 & 0 & \ddots \end{bmatrix} \begin{pmatrix} S_{FYI}^{U235} \\ S_{FYI}^{Pu239} \\ \vdots \end{pmatrix}$$

Table 6. Comparison of S/U and Monte Carlo uncertainty prediction at 60 GWd/TMU. FY uncertainty with “No corr.”

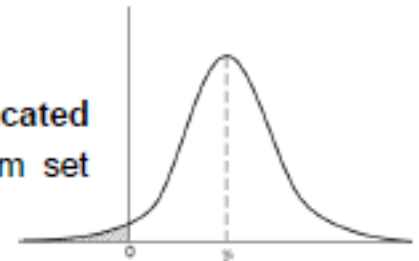
Nuclide	S/U	Monte Carlo
¹⁴⁸ Nd	14.2	13.7
¹³⁷ Cs	1.50	1.50
¹³⁹ La	3.20	3.20

Table 8. Comparison of S/U and Monte Carlo uncertainty prediction at 60 GWd/TMU. FY uncertainty with “No corr.”

Nuclide	S/U	Monte Carlo
¹⁰⁹ Ag	25.0	17.8
¹²⁹ I	20.3	20.7

← WHY?

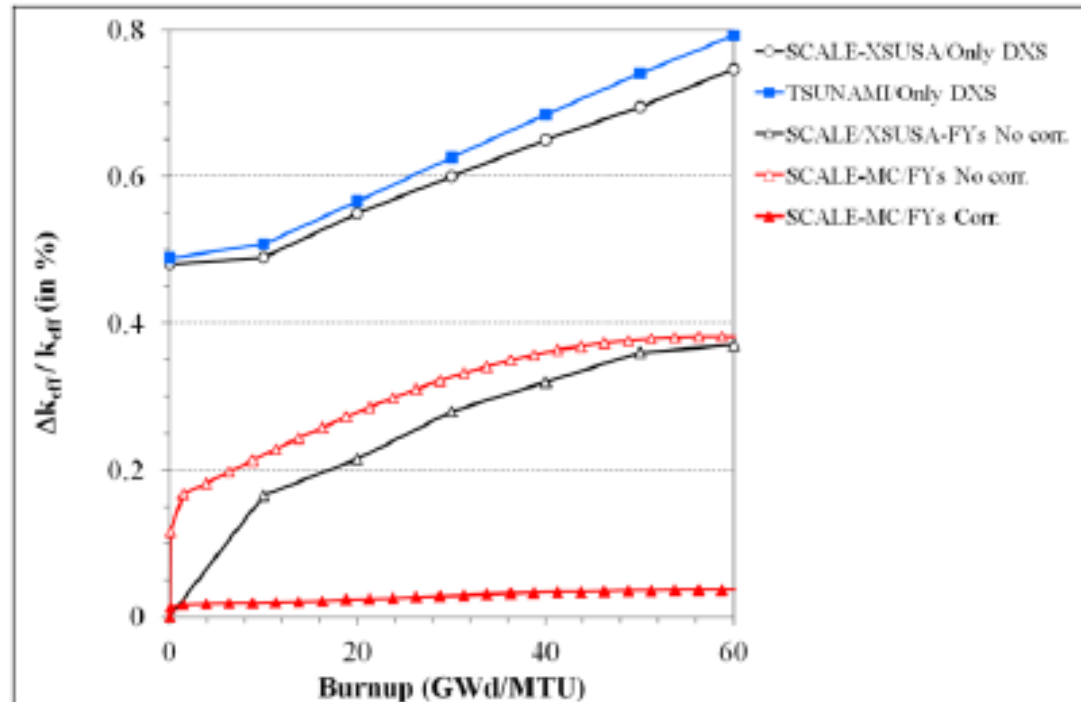
- Our Monte Carlo method uses a “truncated Normal PDF”. Then, the new random set yields a reduced uncertainty.



IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

Figure 5. Relative standard deviation in k_{eff} (in %):

- i) SCALE/XSUSA calculation performed by GRS [7] only uncertainties in cross-section data,
- ii) SCALE/TSUNAMI calculation [2] only uncertainties in cross-section data,
- iii) SCALE/XUSA calculation by GRS with uncertainties only in fission yield data taken from ENDF/B-VII.1/FY data library,
- iv) Monte Carlo with a set of 1000 different fission yield data libraries based on ENDF/B-VII.1 with no-correlation between fission yields ("No corr.")
- v) Monte Carlo with correlations generated by Katakura method in ^{235}U and ^{239}Pu ("Corr.").



$$\text{var}(k) = (S_{\sigma} \quad S_N) \begin{bmatrix} V_{\sigma} & \text{cov}(\sigma, N) \\ \text{cov}(\sigma, N) & V_N \end{bmatrix} \begin{pmatrix} S_{\sigma}^t \\ S_N^t \end{pmatrix} = \text{var}(k_{\sigma}) + \text{var}(k_N) + \text{cov}(k_{\sigma}, k_N)$$

IMPACT OF THE FISSION YIELD COVARIANCE DATA IN BURN-UP CALCULATIONS

- The present study has demonstrated the importance of covariance terms if fission yield data libraries to improve estimations of uncertainties in burn-up applications
- Results in a LWR pin-cell burnup benchmark
- It has been proved that non-correlated independent fission yields data bring to overestimated uncertainties in the number density and criticality predictions
- Comparison between S/U and Monte Carlo shows good agreement (except for ^{109}Ag)
- Assessment of the methodology to generate fission yield covariance data based on Katakura model using information of experimental mass fission yield data
 - ❑ Covariance fission yield data for ^{235}U and ^{239}Pu fissile nuclides were processed
 - ❑ Covariance for isotopes in the same mass chain are modified
 - ❑ Covariance data (by Katakura) changes the criticality and number density uncertainties, reducing its variance to almost a negligible effect (except for ^{109}Ag)

Task 1: Review of current evaluation methods and new requirements

- Had planned to be completed by now.
- Mills to write general summary and short description of JEFF methods by mid-June for email discussion with other participants. Would like 2-3 page summaries from other projects for discussion and final report.

Task 2: Recommendations of new methods and models.

- Rapidly developing subject. Need to focus on report need.

Task 3: Proposal for new fission yield format including covariance.

- Had planned for this year, but need indications from Task 2 first.
- Plan to review work in draft document by Christmas for email discussion.

Final Report

- Produce initial list of contents by end of summer for email discussion.
- After iteration
 - Ask for those who can contribute results, references etc. to each topic
 - Ask for volunteers to write up sections.
- Would like draft distributed early in 2015.

- I feel I have been too passive
- Need to maintain and build momentum in final year.