



Wir schaffen Wissen – heute für morgen

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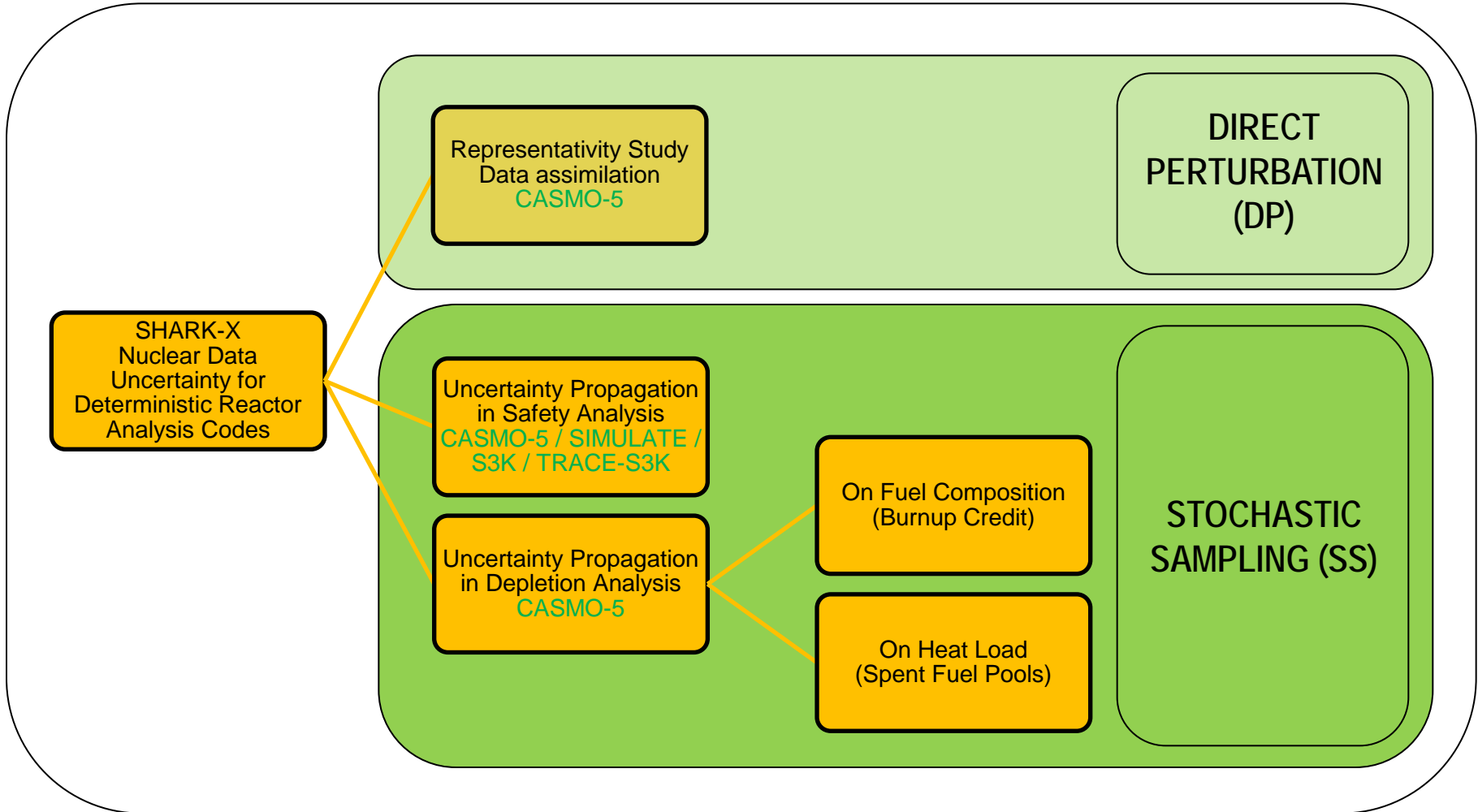
# Status on fission yield perturbation methodology at PSI using CASMO-5



WPEC-37, OECD-NEA, 12<sup>th</sup> May 2014



- 1. INTRODUCTION**
- 2. THE SHARK-X TOOL**
- 3. FISSION YIELD IN CASMO-5**
- 4. ADDING CONSTRAINTS IN THE VCM**
- 5. APPLICATION TO A PWR FUEL ASSEMBLY**
- 6. CONCLUSION**



## 2. THE SHARK-X TOOL

### Recent Development in SHARK-X

**Direct Perturbation (DP) is a brute-force method but provides sensitivity coefficients**

- Select an input parameter for perturbation, e.g. a multigroup cross section  $\sigma_i$
- Perform calculations with perturbed  $\sigma_i$  (e.g.  $\sigma_i \pm 1\%$ ) to estimate the sensitivity coefficient of a response (e.g.  $k_{inf}$ ) with respect to  $\sigma_i$

Sensitivity vector :

$$S_i = \frac{\sigma_i}{k} \frac{\partial k}{\partial \sigma_i}$$

- Fold sensitivity coefficients with input (relative) VCMs to get output uncertainty.

Output Variance :

$$V_{out} = S V_{in} S^T$$

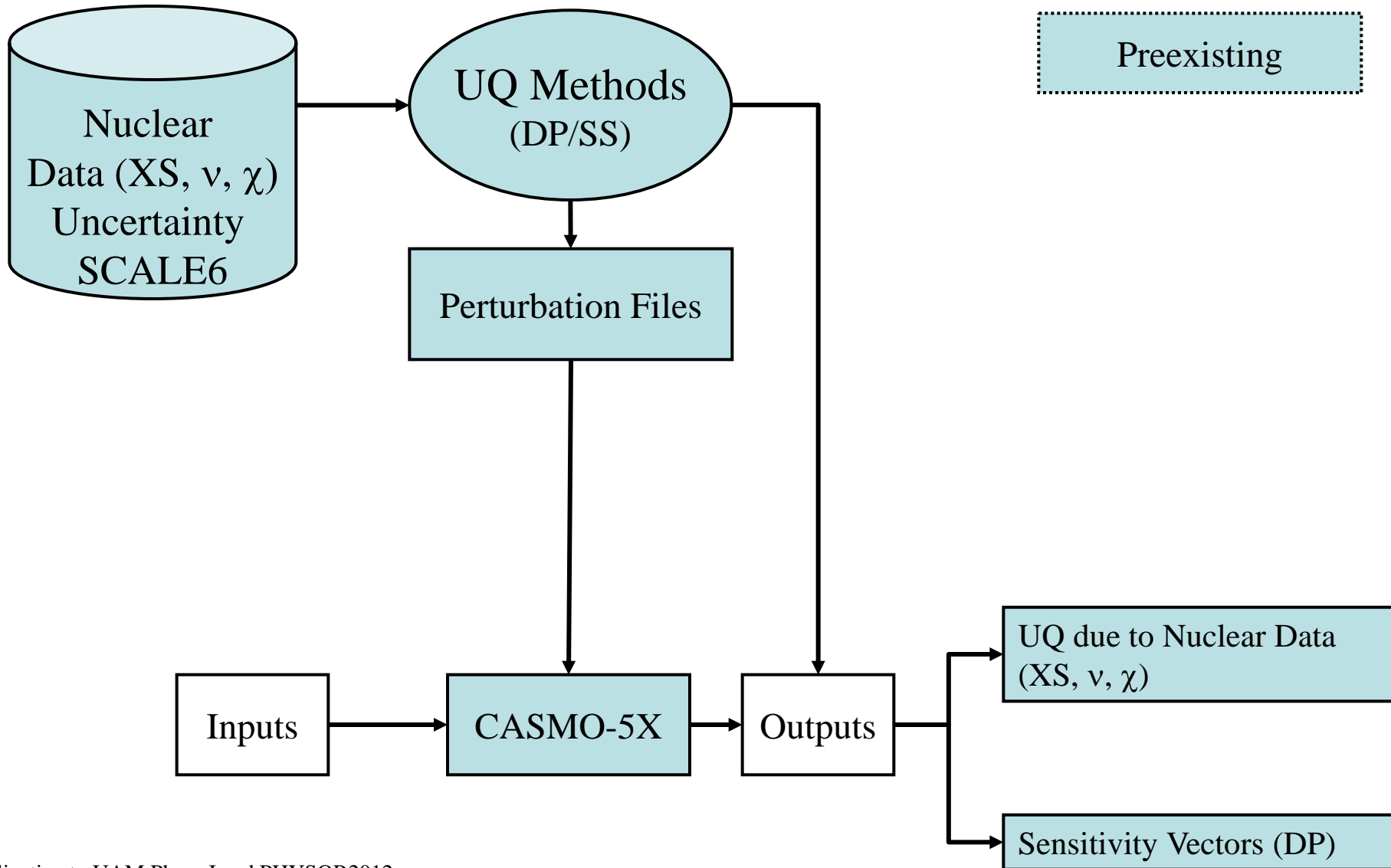
**Statistical Sampling (SS) can handle non-linear systems and general input uncertainties (e.g. non-normally distributed) but does not yield sensitivity information**

- Assume PDFs for all uncertain inputs in model.
- Sample PDFs, respecting covariance of inputs, to generate  $N$  input sets.
- Solve equations (run codes)  $N$  times to generate set of  $N$  outputs.
- Apply statistics to set of responses  $R$  (e.g.  $k_{inf}$  reactivity...) to estimate output variance

**Other approach exist, DP and SS are the only one available with SHARK-X**

## 2. THE SHARK-X TOOL

### Recent Development in SHARK-X

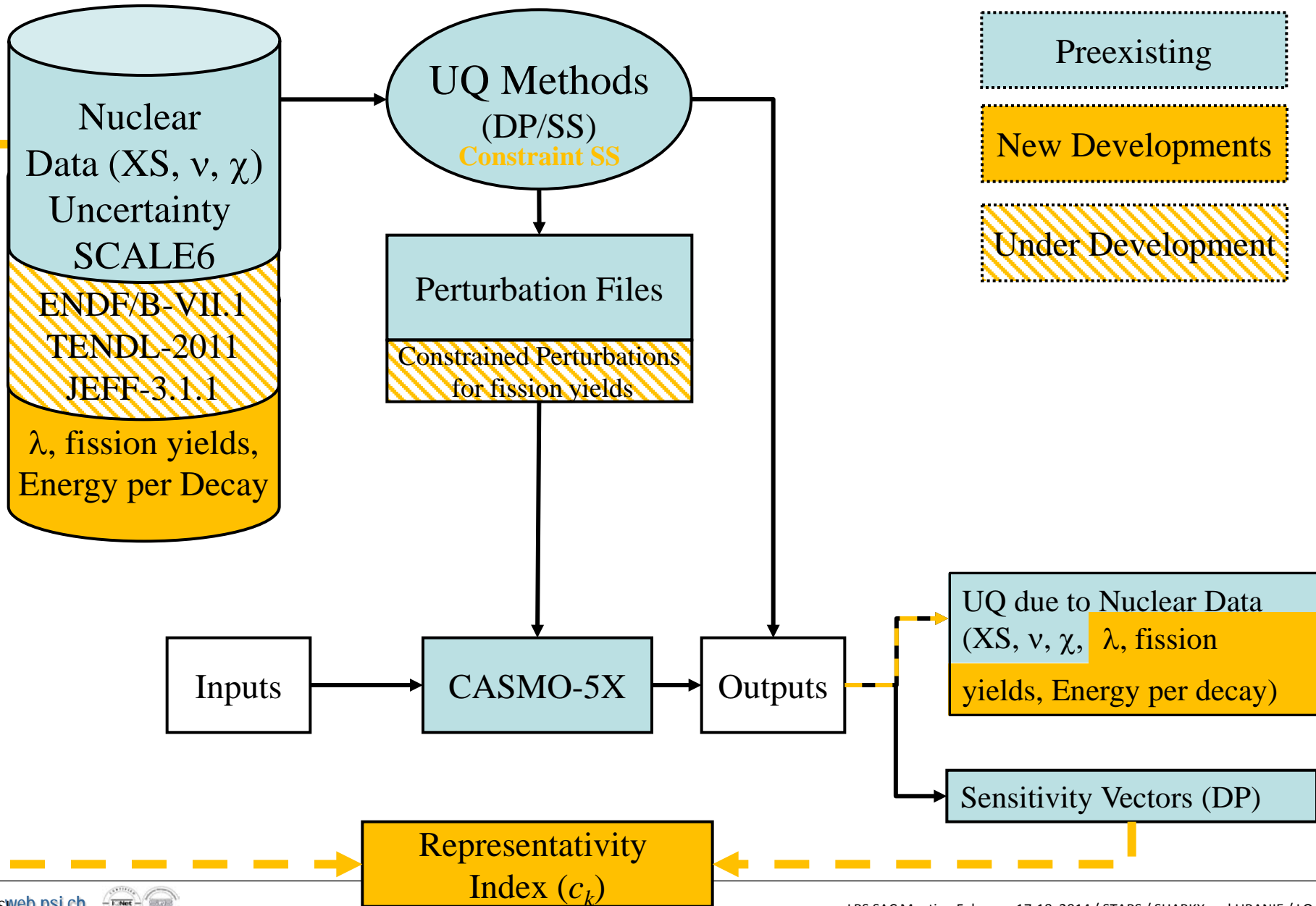


Application to UAM Phase I and PHYSOR2012:

W. Wieselquist, A. Vasiliev, H. Ferroukhi “Nuclear Data Uncertainty Propagation in a Lattice Physics Code using Stochastic Sampling”

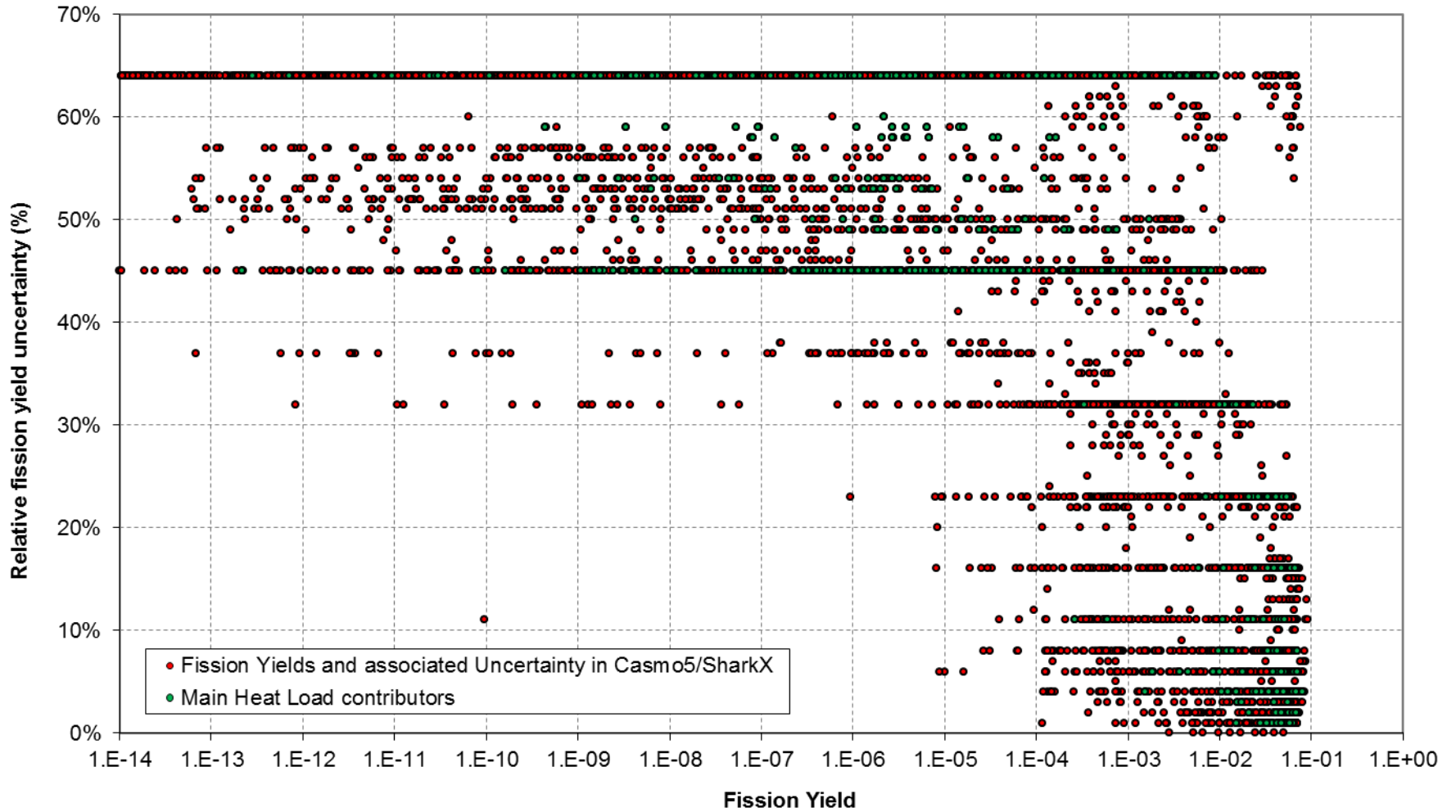
## 2. THE SHARK-X TOOL

### Recent Development in SHARK-X



# 3. FISSION YIELD IN CASMO-5

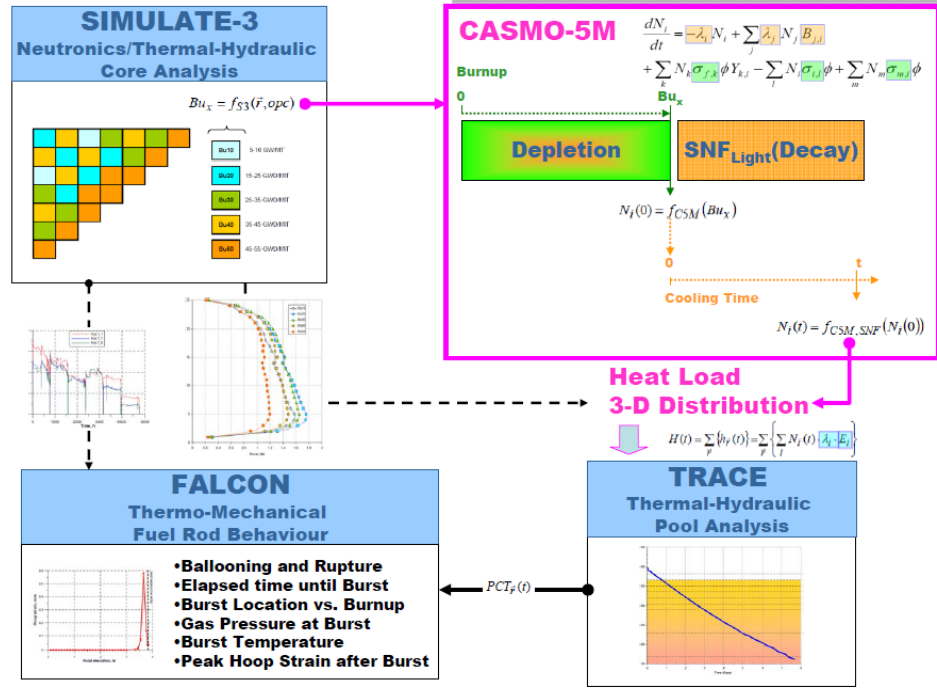
Fission Yield Uncertainty (ENDF-B/VII.1) versus Fission Yield (used in Casmo5)



# 3. FISSION YIELD IN CASMO-5

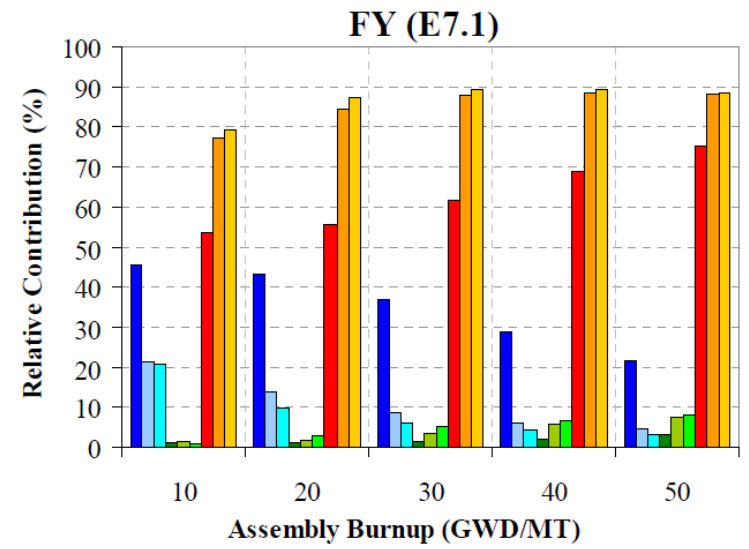
## Spent Fuel Pool Analysis (ENSI On-Call during Fukushima)

- Conducted with Multi-Physics Chain of Best-Estimate Neutronics/T-H/T-M Codes
- **Follow-Up Question:**  
Decay heat uncertainties due to Nuclear Data ?



First Application of SHARK-X for Propagation of Depletion/Decay ND Data

| Days | HL+EPD     | XS           | FY           |
|------|------------|--------------|--------------|
| 4    | Blue       | Green        | Red          |
| 128  | Light Blue | Light Green  | Light Orange |
| 365  | Cyan       | Bright Green | Yellow       |



Contributions to heat load uncertainty.  
The Main impact on Heat Load uncertainty (coming from Nuclear Data) comes from Fission Yields Uncertainty (ENDF/B-VII.1)

Study of Nuclear Decay Data Contribution to Uncertainties in Heat Load Estimations for Spent fuel Pools (H. Ferroukhi, O. Leray, M. Hursin, A. Vasiliev, G. Perret and A. Pautz, Nuclear Data 17/01/2014)

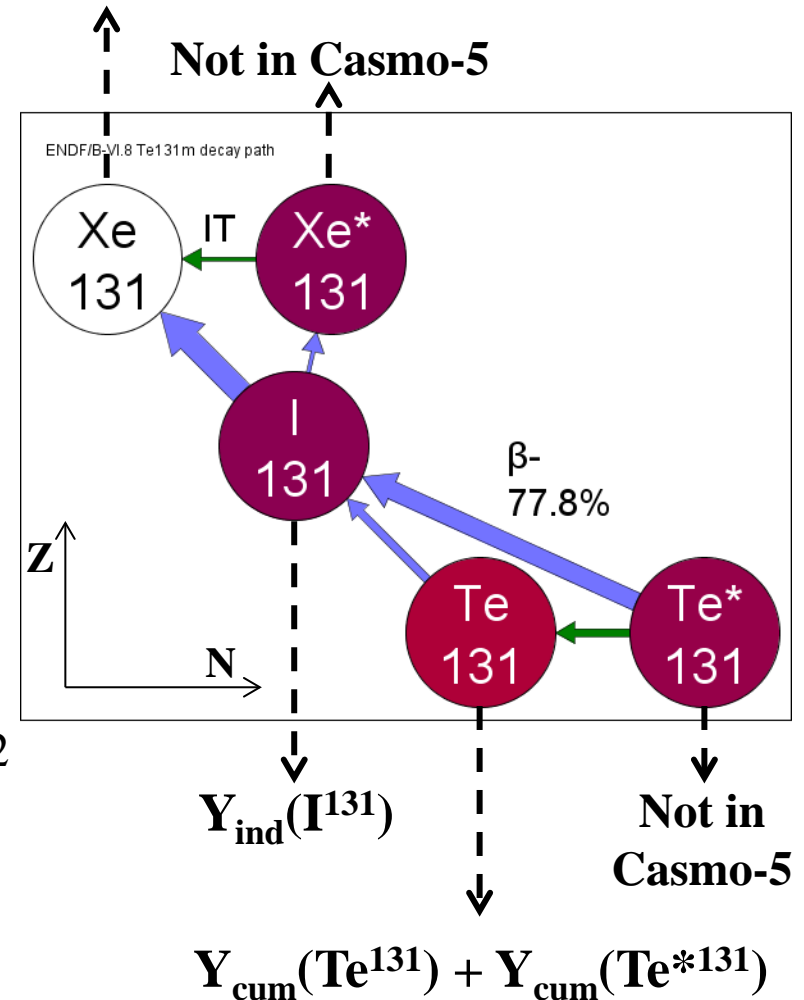
Constraints on Fission Yields :

1. Sum of all fission yield is 2 : 
$$\boxed{\sum_{Z,A} Y(Z, A) = 2}$$
2. Almost the same number of light and heavy FP : 
$$\sum_{Heavy} Y(A) \approx \sum_{Light} Y(A) \approx 1$$
3. Mass conservation :  
(no spontaneous fission) 
$$\sum_{Z,A} A \cdot Y(Z, A) = A_{Father} + 1 - \nu_p$$
4. Z conservation : 
$$\sum_{Z,A} Z \cdot Y(Z, A) = Z_{Father}$$
5. For every Z (not in Casmo) : 
$$\sum_A Y(Z, A) = \sum_A Y(Z_F - Z, A)$$

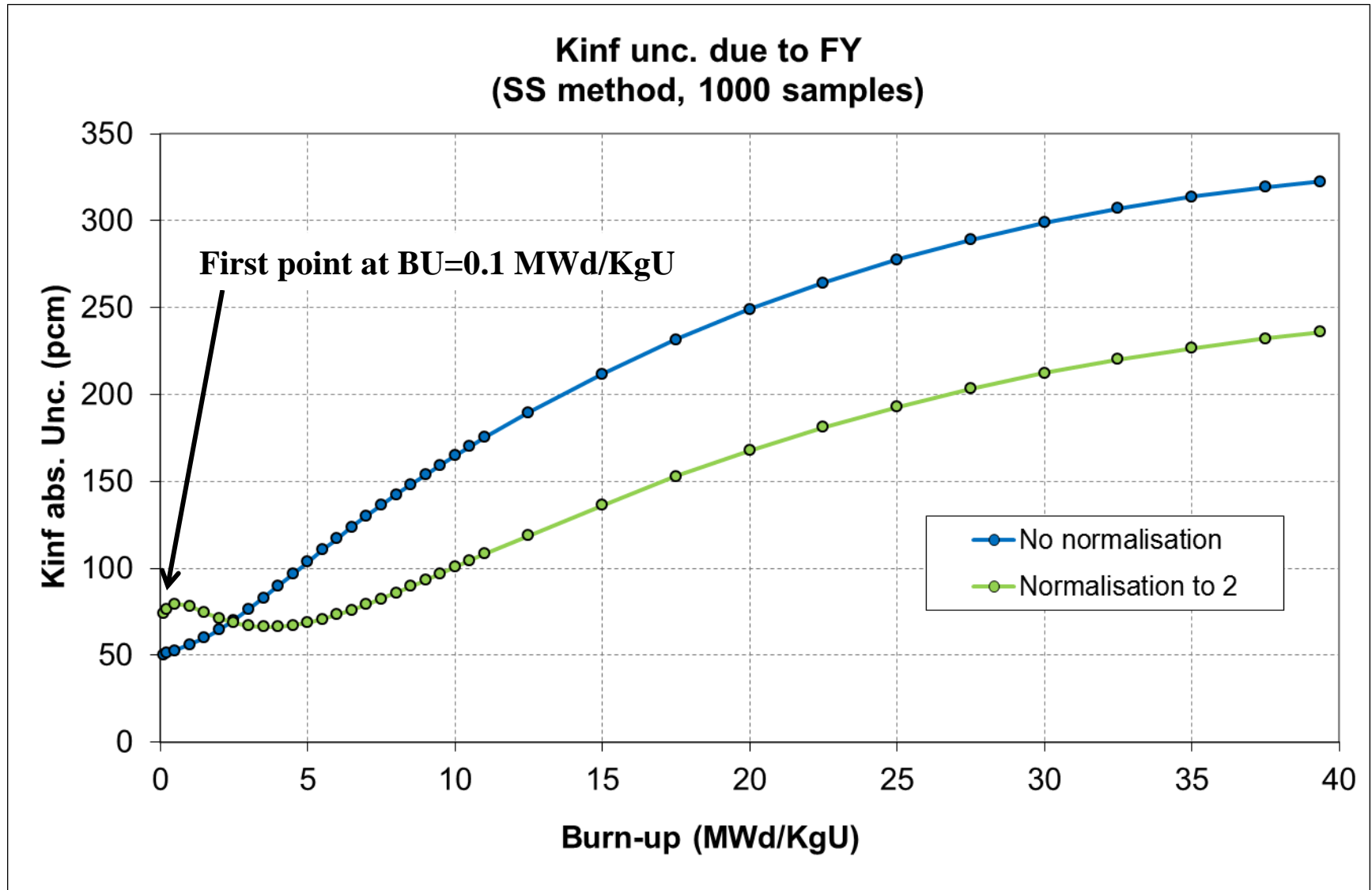
### 3. FISSION YIELD IN CASMO-5

- In Casmo5 fission yields are :
  - Independent fission yields
  - Cumulative fission yields
  - But also some “hybrids” fission yields :
    - Sum of the independent fission yields of the isomers
    - Sum of the cumulative fission yields of the isomers
- 296 isotopes are considered (27 fathers + daughters).
- No perturbation of the branching ratios
- No ternary fission : sum of fission yields is almost 2 (e.g. 1.99865 for  $U^{235}$ )

$$Y_{\text{ind}}(\text{Xe}^{131}) + Y_{\text{ind}}(\text{Xe}^{*131})$$



### 3. FISSION YIELD IN CASMO-5



## 4. ADDING CONSTRAINTS IN THE VCM

The constraints can be satisfied if for every  $Z$ , the sum of the fission yields is kept constant

- For  $d$  daughters and  $p$  elements (e.g. for  $U^{235}$   $d = 215$  and  $p = 35$ ), the sum of fission yield of each given element ( $Z$ ) is  $\lambda_i (\neq 0)$  :

$$\sum_{i=1}^p \lambda_i = 2$$

- $C$  : Condition matrix  $C_{d,p}$  :  $c_{i,j} = 1/\lambda_i$  if  $Z_i$  is the one of the  $j^{\text{th}}$  group,  $c_{i,j} = 0$  otherwise
- $F$  : Fission Yield matrix  $F_{d,p}$  (each row contains the list of the  $d$  fission yields)
- Start from  $M$  (no correlation,  $\sigma$  from ENDF-B/VII.1)

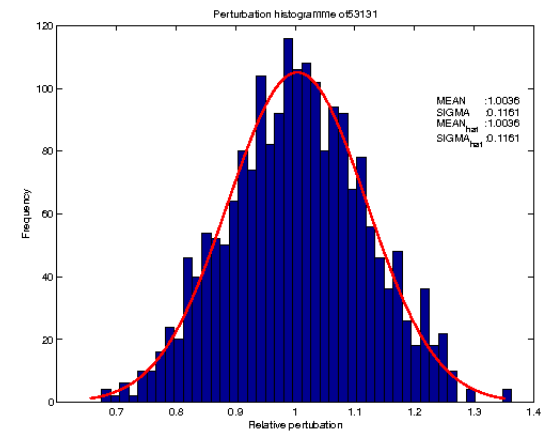
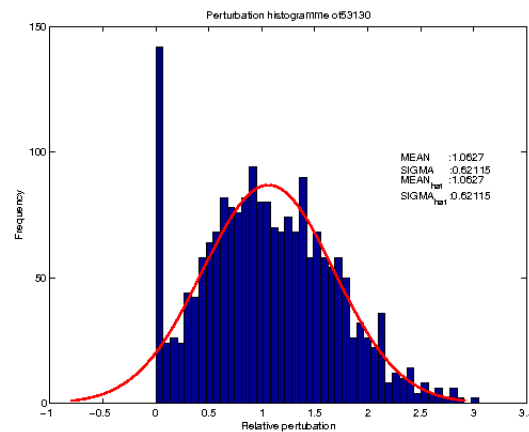
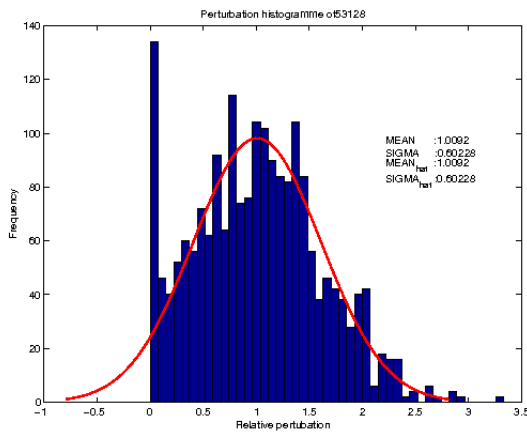
$$C_{d,p} = \begin{matrix} \begin{matrix} \uparrow \\ \mathbf{d} \\ \downarrow \end{matrix} \begin{pmatrix} 1/\lambda_1 & 0 & & & \\ 1/\lambda_1 & 0 & & & 0 \\ 0 & 1/\lambda_2 & & & \\ & & \ddots & & \\ & 0 & & \dots & \\ & & & & 1/\lambda_p \\ & & & & 1/\lambda_p \end{pmatrix} \begin{matrix} \leftarrow \\ \mathbf{p} \\ \rightarrow \end{matrix} \end{matrix} \begin{matrix} \rightarrow \\ \text{Same } Z \end{matrix}$$

$$M_{d,d} = \begin{pmatrix} \sigma_1^2 & & & \\ & \sigma_2^2 & & \\ & & \ddots & \\ & & & \sigma_d^2 \end{pmatrix}$$

$$F_{d,p} = \begin{pmatrix} Y_1 & \dots & Y_1 \\ \vdots & & \vdots \\ Y_d & \dots & Y_d \end{pmatrix}$$

## 4. ADDING CONSTRAINTS IN THE VCM

- Building of the projector  $P$  : 
$$P = I_d - C.F^t$$
- And the normalized Variance-Covariance Matrix : 
$$V = P^t M P$$
- The sampling is then performed using this new  $V$  matrix
- No negative fission yields are allowed (set to 0): It (slightly) changes the normalisation !



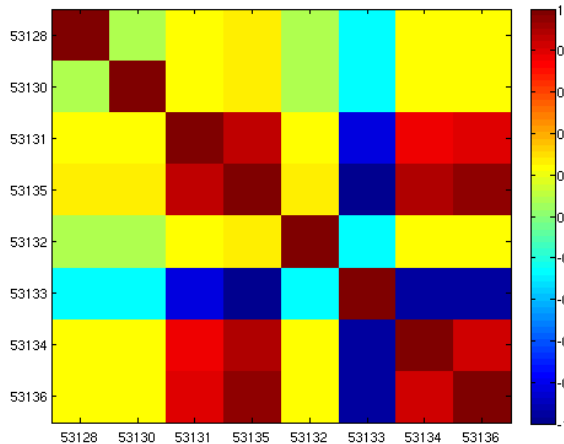
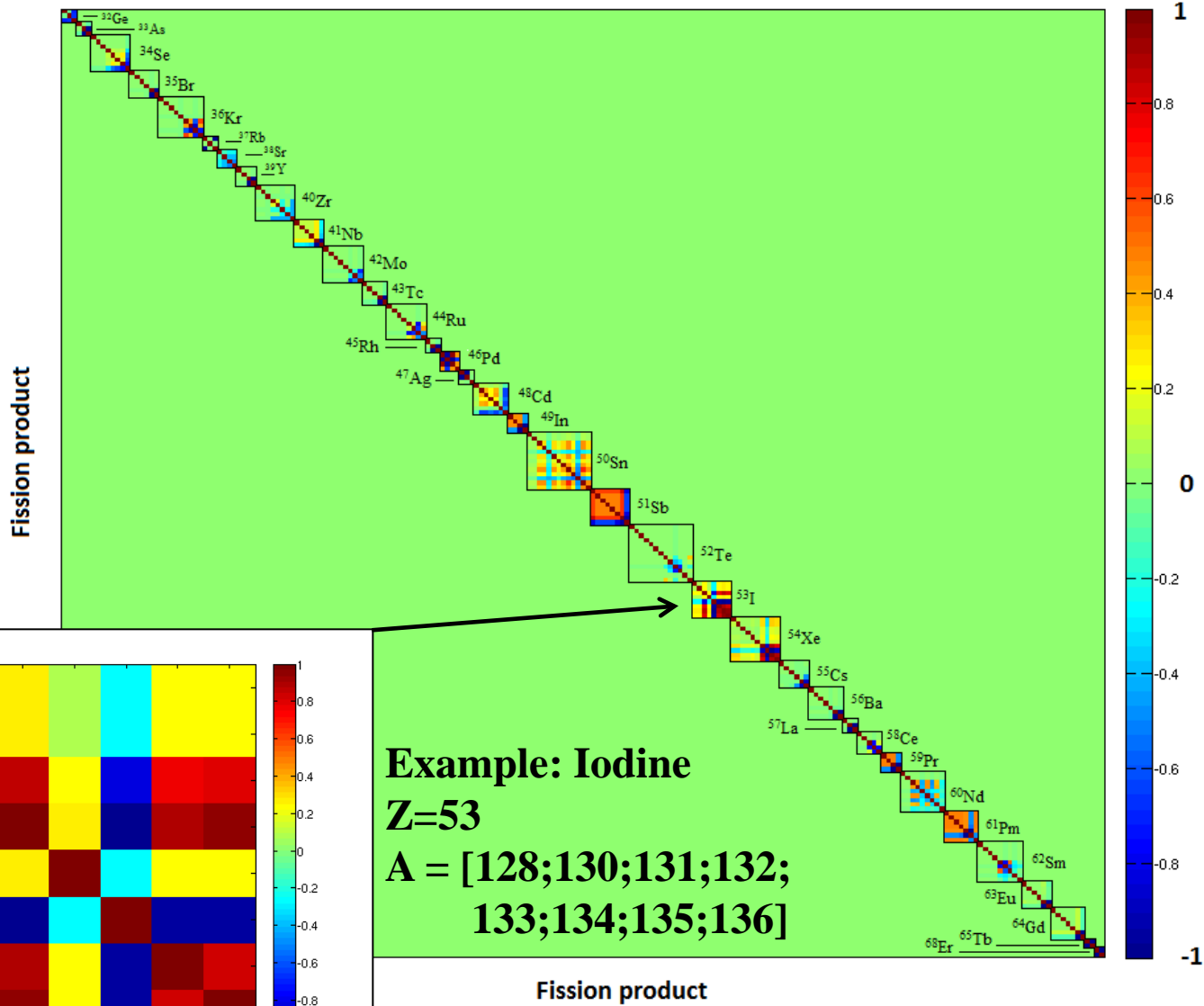
- From the  $V$  matrix, a correlation matrix can be retrieved

Application of this methodology to spent fuel nuclide composition was submitted to PHYSOR2014:

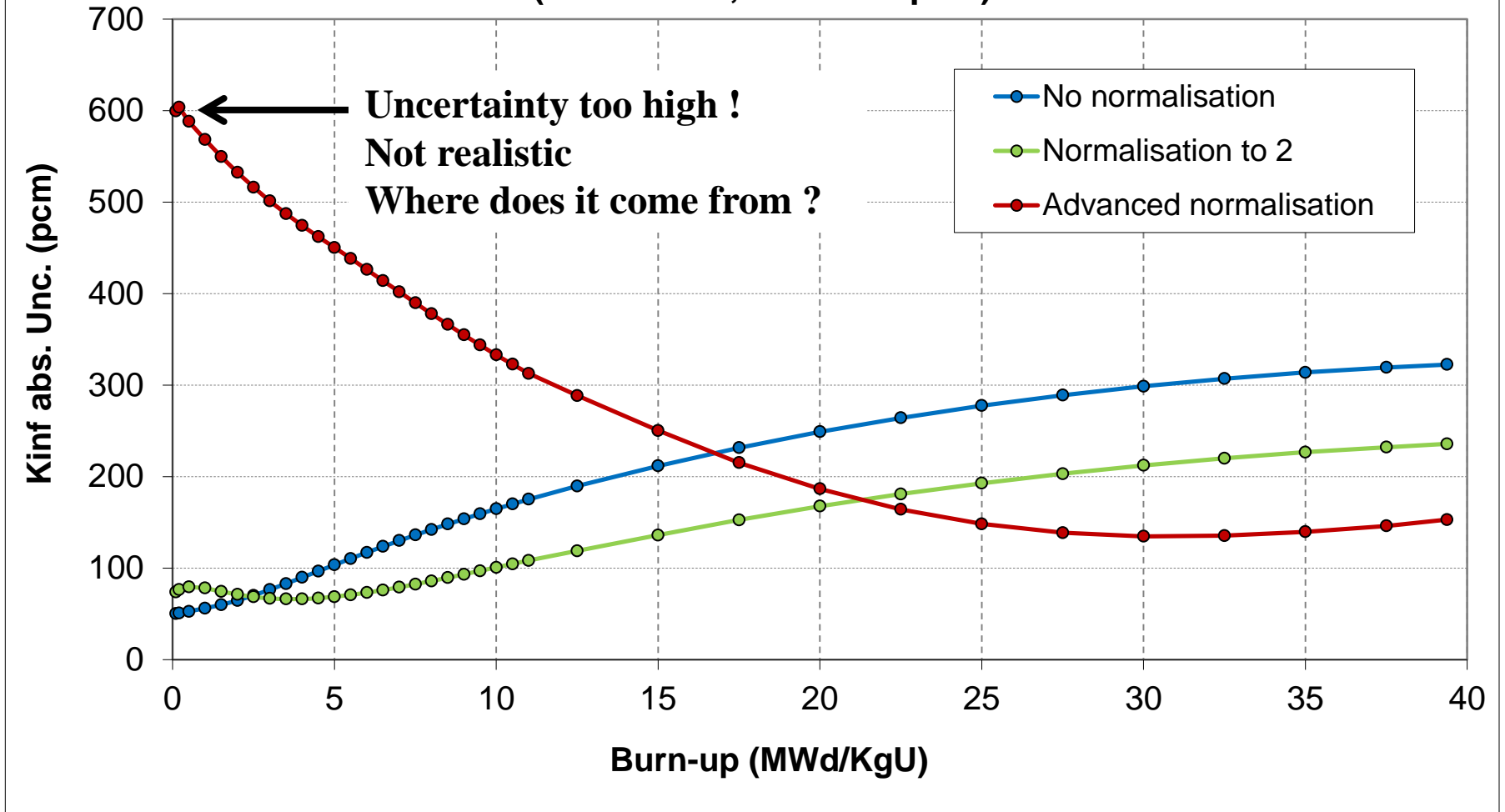
O. Leray, P. Grimm, M. Hursin, H. Ferroukhi and A. Pautz “Uncertainty Quantification of Spent Fuel Nuclide Compositions due to Cross Sections, Decay Constants and Fission Yields”

# 4. ADDING CONSTRAINTS IN THE VCM

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



**Kinf unc. due to FY  
(SS method, 1000 samples)**

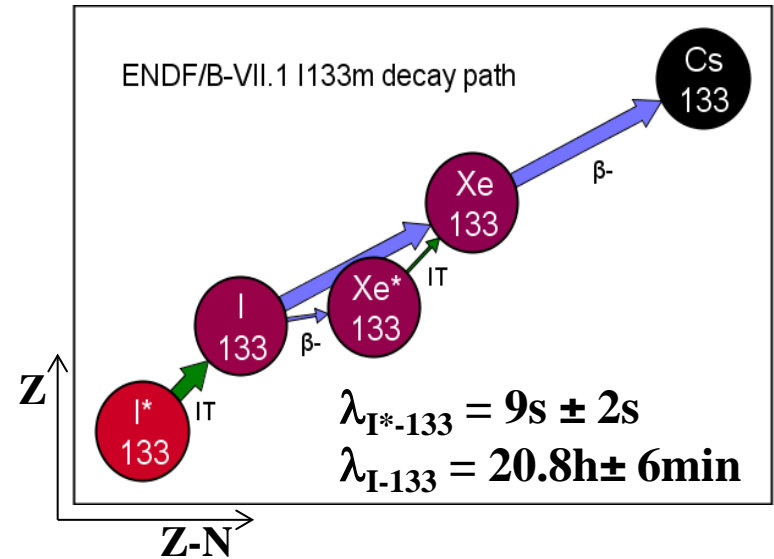


Isotope : 53-I-133

CUMULATIVE Fission Yield from U235

| Evaluation     | Fission Yield | Abs. Std   | Rel. Std |
|----------------|---------------|------------|----------|
| ENDF-B/VI.8    | 6.6965E-02    | 4.2858E-02 | 64.00%   |
| ENDF-B/VII.0   | 6.6965E-02    | 4.2858E-02 | 64.00%   |
| ENDF-B/VII.1   | 6.6965E-02    | 4.2858E-02 | 64.00%   |
| JEF-2.2        | 6.6128E-02    | 8.8307E-04 | 1.34%    |
| JEFF-3.1       | 6.5948E-02    | 1.0550E-03 | 1.60%    |
| JEFF-3.1.1     | 6.5948E-02    | 1.0550E-03 | 1.60%    |
| JENDL-3.3      | 6.6991E-02    | 0          | 0.00%    |
| JENDL-4.0      | 6.6868E-02    | 4.2796E-02 | 64.00%   |
| JENDL/FPY-2011 | 6.6881E-02    | 4.2804E-02 | 64.00%   |
| RUSFOND-2010   | 6.5948E-02    | 1.0550E-03 | 1.60%    |
| TENDL-2011     | 6.6965E-02    | 4.2858E-02 | 64.00%   |
| GEFY-3.3       | 5.0814E-02    | 6.1370E-03 | 12.08%   |

Source: Janis



## Why such a discrepancy ?

For ENDF-B evaluations, the reference is:

T. R. England, B. F. Rider "Evaluation and Compilation of Fission Product Yields", Los Alamos National Laboratory, LA-UR-94-3106 ENDF-349, October 1994

**One can find for (U<sup>235</sup> thermal fission) Mass chain A = 133, FY = 6.99915 and sigma = 0.35 % !**

For JEFF evaluations, the reference is:

R. W. Mills "Fission product yield evaluation", Ph.D. Thesis, University of Birmingham, March 1995

**From 7 experiments, an uncertainty of 3% is assessed**

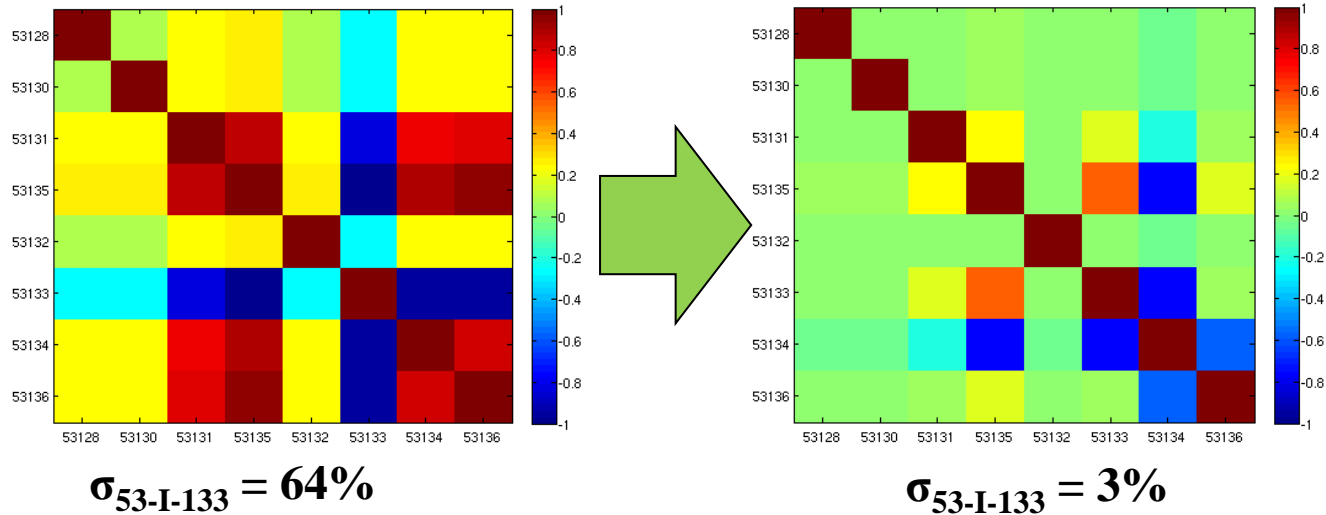
(but using the Chi square test, it is recommended to take largest value between internal and external Std. of the whole mass chain A=133 which is 1.5%)

Sensitivity analysis with 3% uncertainty (Why std=1.6% in JEFF-3.1.1 ?)

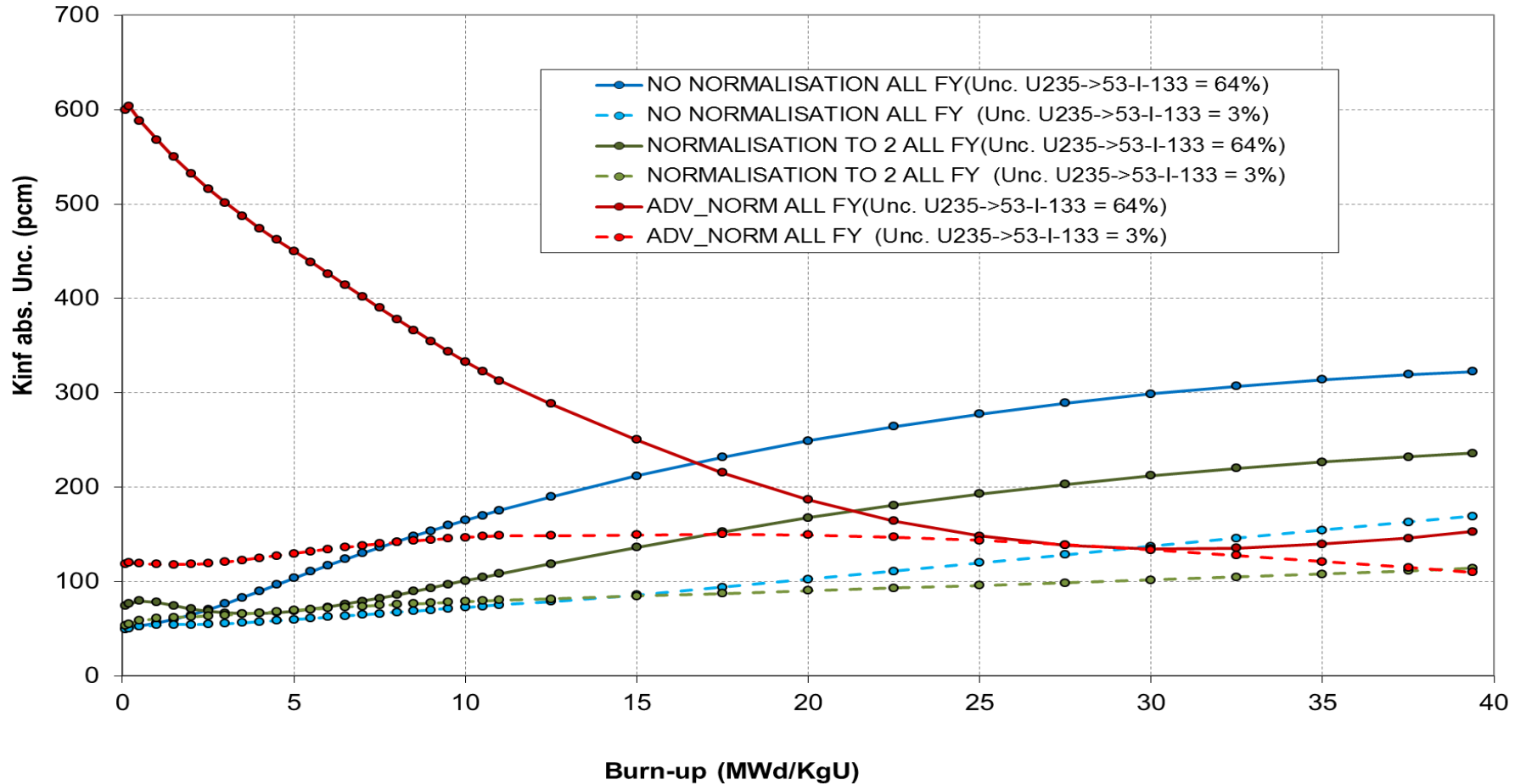
Z = 53 Iodine

| A            | 128 | 130 | 131 | 132 | 133      | 134 | 135 | 136 |
|--------------|-----|-----|-----|-----|----------|-----|-----|-----|
| $\sigma$ (%) | 64  | 64  | 11  | 64  | <b>3</b> | 8.6 | 1.4 | 6   |

### Z=53 Correlation Matrix



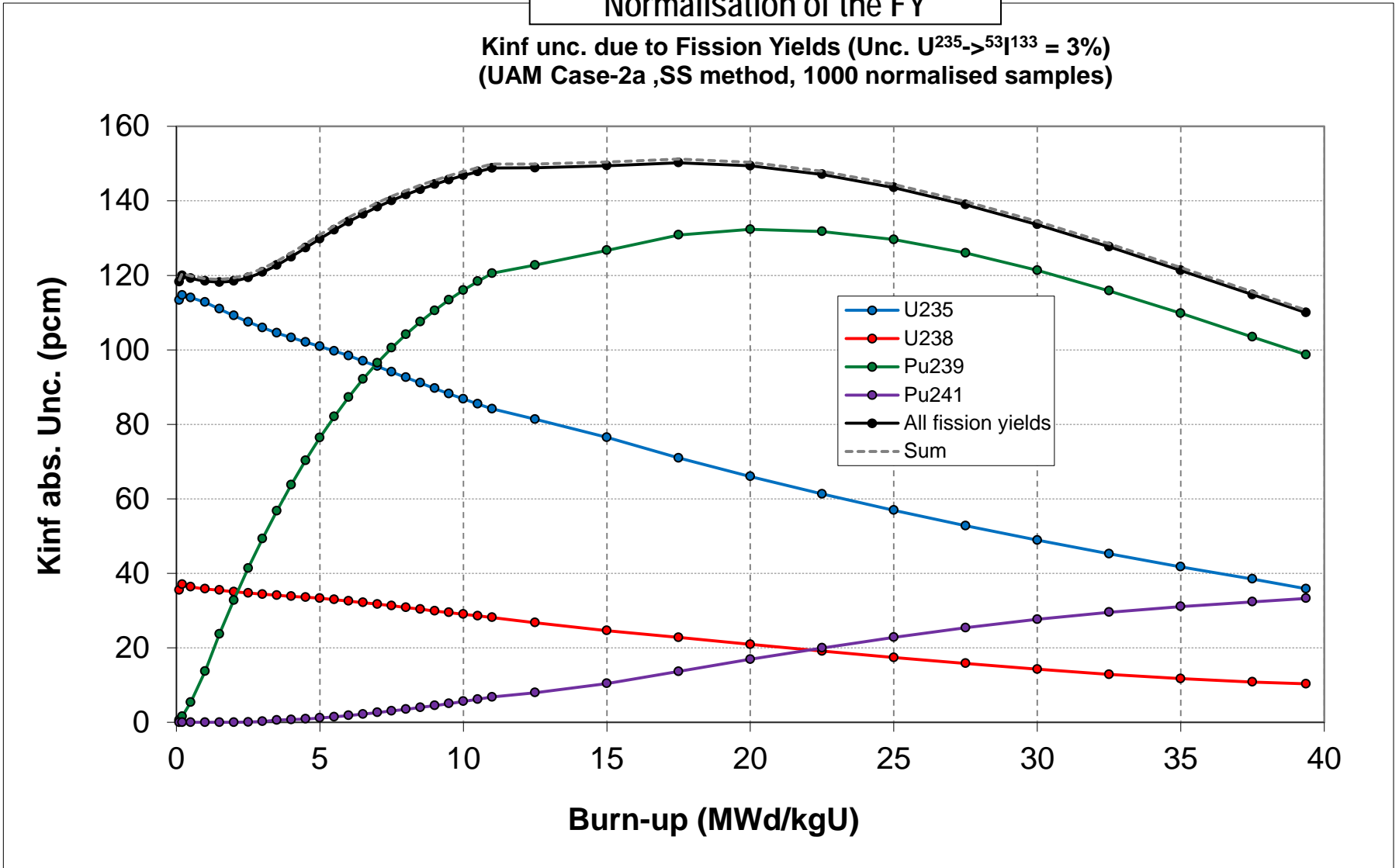
Kinf Uncertainty due to FY and sensitivity to the  $U^{235} \rightarrow I^{133}$  FY  
(SS method, 1000 samples)



# 5. APPLICATION TO A PWR FUEL ASSEMBLY

Normalisation of the FY

Kinf unc. due to Fission Yields (Unc.  $U^{235} \rightarrow ^{53}I^{133} = 3\%$ )  
(UAM Case-2a ,SS method, 1000 normalised samples)



## 6. CONCLUSION

- Limitations of CASMO-5:
  - Decay chains simplified (ind. FY + cum. FY)
  - Branching ratios simplified (possibility to have access to 41 BR only)
  - As a consequence: Impossible to change FY library (only ENDF/B-VII.0)
- Normalisation of the FY:
  - Basic normalisation to 2 (no ternary fission)
  - The constraint by element implies that the FY are only element dependent
  - Need for a more advanced technique
- The Kinf can be very sensitive to the FY (e.g.  $U^{235}$  to  $I^{133}$ )
  - Need improvement of reliable fission yield uncertainty
  - Improvement of the FY normalisation in CASMO-5 (using GEF?)
- Next step
  - Assessment and comparison of the results within the UAM Phase II Benchmark

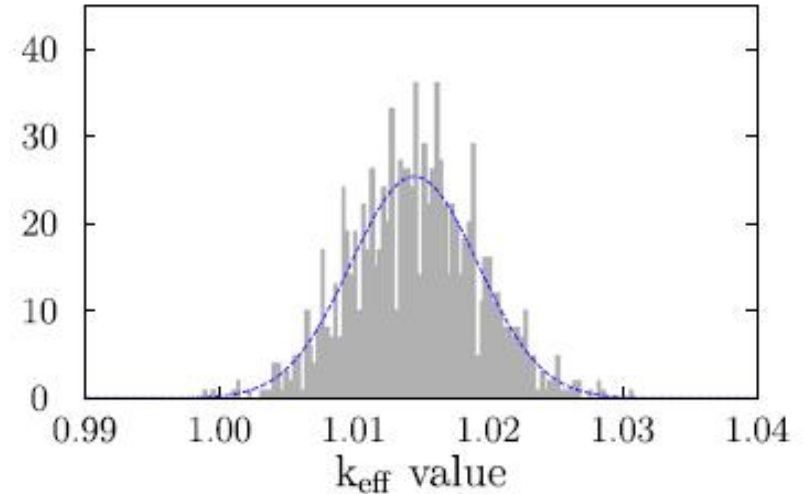
THANK YOU FOR YOUR ATTENTION



# 7. Back-up slides

**Stochastic Sampling (SS)** can handle non-linear systems and general input uncertainties but does not directly give sensitivity information

1. Assume PDFs for all uncertain inputs in model. For Nuclear Data uncertainty propagation, variance-covariance matrices (VCMs) implies a multi-variate normal distribution.
2. Sample PDFs, respecting covariance of inputs, to generate N input sets.
3. Solve equations (run codes) N times to generate set of N outputs.
4. Apply statistics to set of responses R to estimate output variance



INPUT SAMPLE of Size  $N$

$$\begin{pmatrix} (\mathbf{X})_1 \\ (\mathbf{X})_2 \\ \vdots \\ (\mathbf{X})_N \end{pmatrix} \equiv \begin{pmatrix} (X_1 \dots X_K)_1 \\ (X_1 \dots X_K)_2 \\ \vdots \\ (X_1 \dots X_K)_N \end{pmatrix}$$

Input Multivariate  $\mathbf{X}$

Assign Values  
to input:  
Sampling Process

$$\begin{pmatrix} (x_1 \dots x_K)_1 \\ (x_1 \dots x_K)_2 \\ \vdots \\ (x_1 \dots x_K)_N \end{pmatrix}$$

$K$  Input Sampled Values for  $N$  runs

$$\begin{pmatrix} \text{Code}((x_1 \dots x_K)_1) \\ \text{Code}((x_1 \dots x_K)_2) \\ \vdots \\ \text{Code}((x_1 \dots x_K)_N) \end{pmatrix} \equiv \begin{pmatrix} (y_1 \dots y_M)_1 \\ (y_1 \dots y_M)_2 \\ \vdots \\ (y_1 \dots y_M)_N \end{pmatrix} \equiv \begin{pmatrix} (\mathbf{Y})_1 \\ (\mathbf{Y})_2 \\ \vdots \\ (\mathbf{Y})_N \end{pmatrix}$$

$M$  Output Variables for  $N$  Runs

OUTPUT SAMPLE of Size  $N$

# 7. Back-up slides

|    | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|----|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|
| 1  | - | - | - | - | - | - | - | - | - | -  | -  | -  | -  | -  | -  |
| 2  | - | g | - | - | - | - | - | - | - | -  | -  | -  | -  | g  | -  |
| 3  | - | - | - | - | G | - | - | - | G | -  | -  | -  | -  | -  | -  |
| 4  | - | - | - | G | - | - | - | - | - | -  | G  | -  | -  | -  | -  |
| 5  | - | - | - | - | - | - | - | - | - | -  | -  | -  | -  | -  | -  |
| 6  | - | - | G | - | G | - | - | - | G | -  | -  | G  | -  | -  | -  |
| 7  | - | - | - | - | - | - | - | - | - | -  | -  | -  | -  | -  | -  |
| 8  | - | - | - | - | - | - | I | - | - | -  | -  | -  | -  | -  | -  |
| 9  | - | - | - | - | - | - | - | - | - | -  | -  | -  | -  | -  | -  |
| 10 | - | - | G | - | G | - | - | - | G | -  | -  | G  | -  | -  | -  |
| 11 | - | - | - | - | - | - | - | - | - | -  | -  | -  | -  | -  | -  |
| 12 | - | - | - | G | - | - | - | - | - | -  | G  | -  | -  | -  | -  |
| 13 | - | - | - | - | G | - | - | - | G | -  | -  | -  | -  | -  | -  |
| 14 | - | g | - | - | - | - | - | - | - | -  | -  | -  | -  | g  | -  |
| 15 | - | - | - | - | - | - | - | - | - | -  | -  | -  | -  | -  | -  |

Figure 19: TMI-1 FA Pin Layout

Table 47: TMI-1 FA Pin Descriptions

| Marker | Rod Type                  |
|--------|---------------------------|
| g      | 2.0 w/o Gd 4.12% 235U pin |
| G      | Guide Tube                |
| I      | Instrumentation Tube      |
| -      | 4.12% 235U fuel pin       |

Table 48: TMI-1 FA Details

|                         |           |
|-------------------------|-----------|
| FA Pitch                | 218.1 mm  |
| Active Height           | 3657.6 mm |
| # Guide Tubes           | 16        |
| # Instrumentation Tubes | 1         |
| # 2.0 w/o Gd pins       | 4         |
| # 4.12% 235U pins       | 204       |
| Total rods/FA           | 225       |

## UAM-Phase II Benchmark (Case2a)

Table 49: TMI-1 Fuel, Guide, and Instrumentation Rod Dimensions and Parameters

|                         |           |
|-------------------------|-----------|
| Cladding OD             | 10.922 mm |
| Cladding ID             | 9.58 mm   |
| Cladding Thickness      | 0.673 mm  |
| Pin Pitch               | 14.427 mm |
| Fuel Pellet OD          | 9.390 mm  |
| Fuel Pellet Height      | 11.4 mm   |
| % Density               | 93.8% TD  |
| Guide Tube OD           | 13.462 mm |
| Guide Tube ID           | 12.649 mm |
| Instrumentation Tube OD | 12.522 mm |
| Instrumentation Tube ID | 11.201 mm |

Table 50: TMI-1 Core Boundary Conditions

|                        |                |
|------------------------|----------------|
| Core Power             | 2772 MWt       |
| Coolant Temperature    | 578 K          |
| Core Pressure          | 15.51 MPa      |
| Core Coolant Flow Rate | 16052.4 kg/sec |

Table 52: TMI-1 Irradiation History

| Time | Power |
|------|-------|
| Days | MW/t  |
| 875  | 45.00 |

**Calculation with CASMO5-X, 19 Energetic Groups at Hot Full Power**

# 7. Back-up slides

| Fissionable isotopes taken into account in SHARK-X |            |
|--|------------|
| ENDF/B-VII.1                                       | JEFF-3.1.1 |
| 90232  | 90232      |
| 91231  |            |
| 92232  |            |
| 92233  | 92233      |
| 92234  | 92234      |
| 92235  | 92235      |
| 92236  | 92236      |
| 92237  |            |
| 92238  | 92238      |
| 93237  | 93237      |
| 93238  | 93238      |
| 94238  | 94238      |
| 94239  | 94239      |
| 94240  | 94240      |
| 94241  | 94241      |
| 94242  | 94242      |
| 95241  | 95241      |
| 95243  | 95243      |
| 95601  | 95601      |
| 96242  |            |
| 96243  | 96243      |
| 96244  | 96244      |
| 96245  | 96245      |
| 96246  |            |
| 96248  |            |
| 98249  |            |
| 98251  |            |