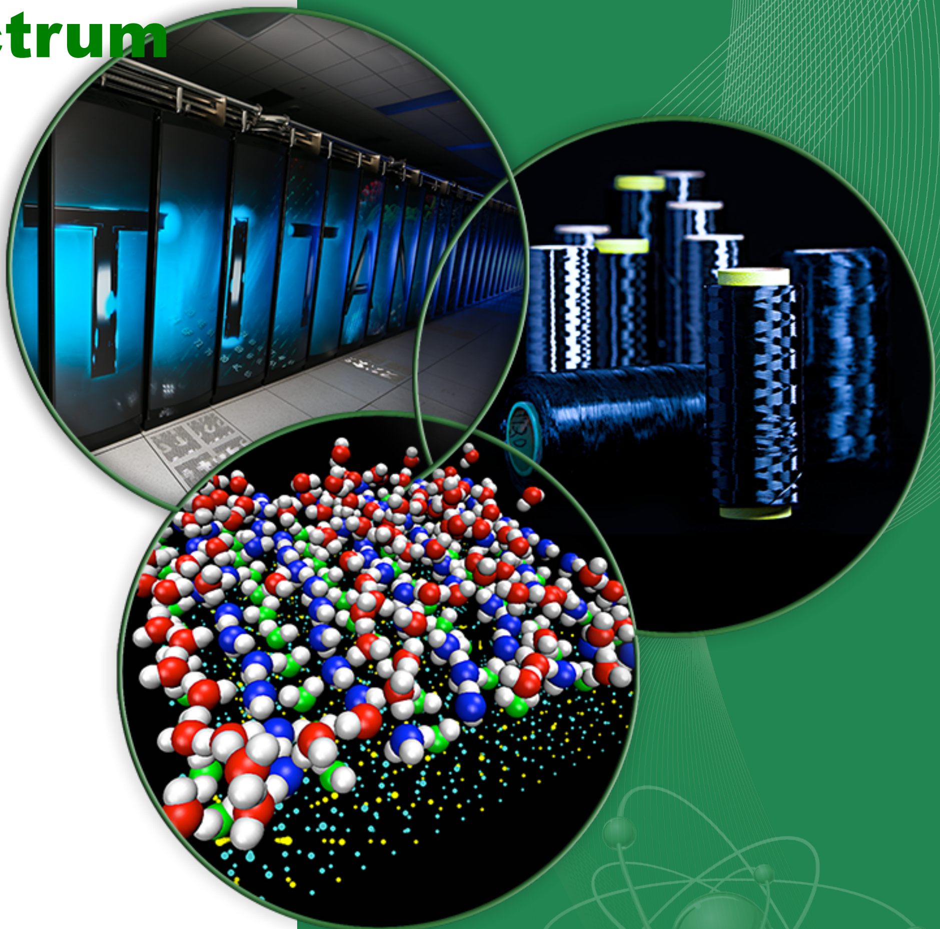
FPY Covariance Matrices in the Thermal and Fission Spectrum Energy Range



M.T. Pigni, M.W. Francis, I.C. Gauld
Oak Ridge National Laboratory
Oak Ridge, TN

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Outline

- **Growing interest in covariance data for fission product yield (FPY)**
- **Status of ENDF/B-VII.1 FPY sub-library**
- **Inconsistencies between Indep.(MT=454)/Cum.(MT=459) FPY and decay data (MT=457)**
- **Methodology to estimate independent FPY and related covariance data**
- **Results (independent/cumulative) for noble gases (krypton and xenon)**
- **Conclusions and future work**

Introduction

- **In 2012 ORNL started a project to develop and investigate methodologies to generate FPY covariance data**
  - **Step 1 :** generate covariance library for nuclear decay and fission yield data
    - compile uncertainties for nuclear *decay* and *fission yields* data
    - develop methods to generate related covariance matrices
  - **Step 2 :** Monte Carlo-based uncertainty methods developed for analysis of covariance matrices will be used to generate perturbed covariance libraries developed in Step 1 (SAMPLER)
  - **Applications :** demonstrate the feasibility of the project on applications, i.e. fuel decay heat, radio toxicity, burn up credit analysis
    - Ind. FPY uncertainties in ENDF too large (e.g. ^{148}Nd)
- **In 2013 first results for n+^{235}U at thermal**
  - Covariance matrix generated on the basis of Wahl and Gaussian semi empirical model using ENDF/B-VII.1 uncertainties
  - Covariance matrix generated by retroactive Bayesian with updated uncertainties
- **In 2014 results on n+^{235}U(thr,500keV,14MeV), ^{239,241}Pu(thr),^{238}U(500keV)**
  - FPY cov. data needed by Defense Threat Reduction Agency (DTRA) project
  - Motivated to improve prediction on noble gases (Kr and Xe) cumul. FPYs
  - Methodology : sequential Bayesian (T. Kawano)

FPY sub-library in ENDF/B-VII.1

#	Nuclei	Year	Author(s)
1	$^{227,229,232}Th$	1994	England et al. [1994]
2	^{231}Pa	1994	England et al. [1994]
3	$^{232\text{-}238}U$	1994	England et al. [1994]
4	$^{237,238}Np$	1994	England et al. [1994]
5	$^{238\text{-}242}Pu$	1994/2011	England [1994]/Chadwick [2011]
6	$^{241,242m,243}Am$	1994	England et al. [1994]
7	$^{242\text{-}248}Cm$	1994	England et al. [1994]
8	$^{249,251}Cf$	1994	England et al. [1994]
9	^{254}Es	1994	England et al. [1994]
10	^{255}Fm	1994	England et al. [1994]

In 1993 T. R. England and B. F. Rider produced a recommended set of *independent* and *cumulative* yields for the fission products based on a compiled list of open literature measurements and calculated charge distributions.

Except for ^{239}Pu, England and Rider FPY evaluations are still in ENDF/B-VII.1 library, but …
…since 1993 decay sub-library data (branching ratios) updated!!

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Decay Data & (Stable) Cumulative FPY

Black dots : ratio of cumulative FPYs obtained by independent FPY and decay data in ENDF/B-VII.1 to cumulative FPYs in ENDF/B-VII.1.

Although deviations are small, **ratios should be one!!**

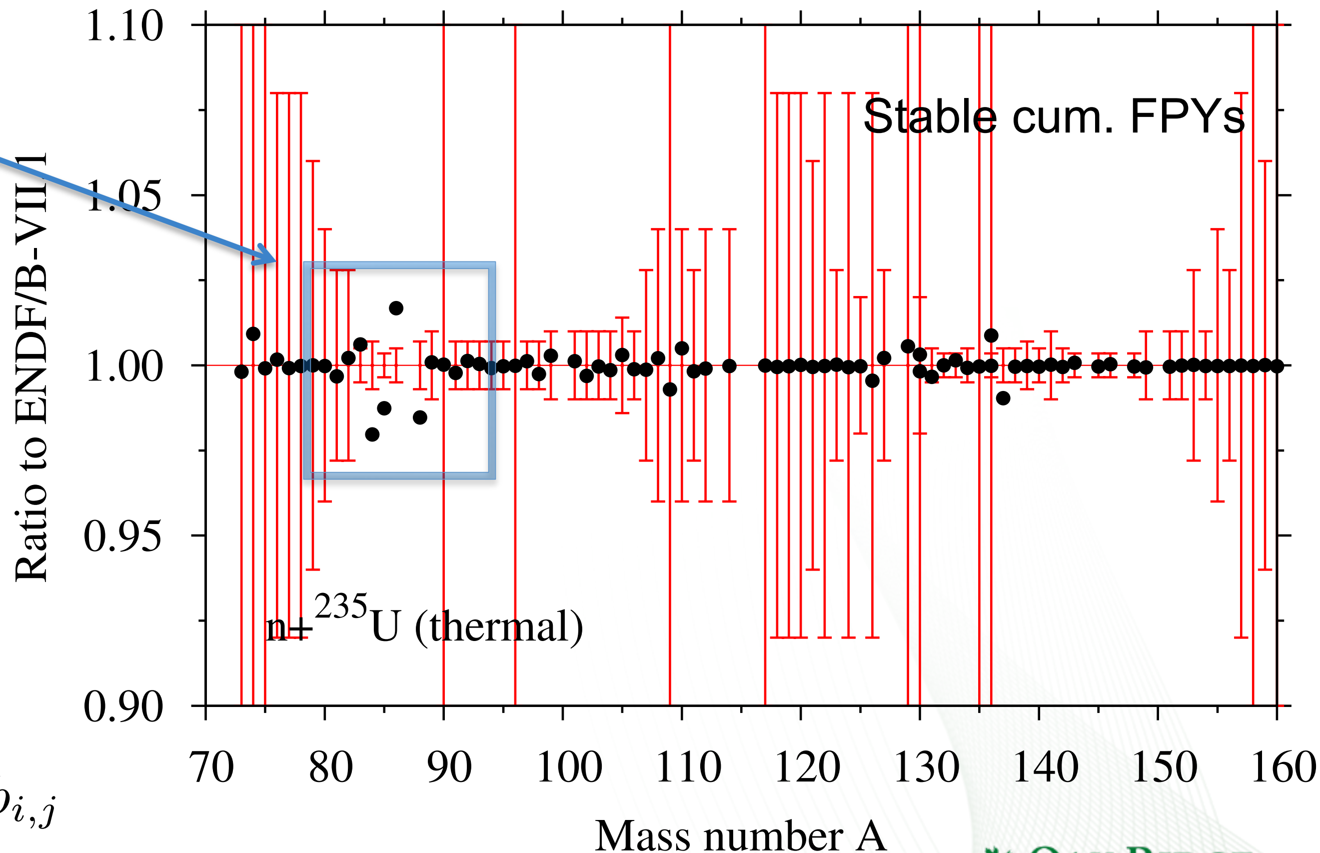
In red uncertainties (%) of cumulative yields in ENDF/B-VII.1

Biggest deviations

Cumulative yields

Independent FPY

Branching ratios



$$C_i(\mathbf{I}) = I_i + \sum_{j \in \mathbf{k}^i} C_j(\mathbf{I})\ b_{i,j}$$

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Sequential Bayesian Method (Kawano)

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

$$\vec{I}_1 = \vec{I}_0 + P_1 S^t Z^{-1} [\vec{\varsigma} - \vec{C}(\vec{I}_0)]$$

I is vector of ind. FPY (parameters)

We considered each cum. FPY
Not only long lived ones

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

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

$$\vec{T}^t \vec{I} = \sum_i T_i I_i = 2$$

Constraint I : total yield sums to 2

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

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

$$\vec{U}^t I = \sum_i A_i I_i = A_f - \nu$$

Constraint II on the mass number

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

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

$$\vec{V}^t \vec{I} = \sum_i Z_i I_i = Z_f$$

Constraint III on the charge number

Example of S-matrix for Krypton

The relation between cum. and ind. defines a set of weighted linear coupled equations.
The coupling is from delayed neutron emissions (also alpha if included)

^{87}Ge	^{87}As	^{87}Se	^{87}Br	^{86}Ga	^{86}Ge	^{86}As	^{86}Se	^{86m}Br	^{86}Br	^{86}Kr	^{85}Ga	^{85}Ge	^{85}As	^{85m}Se	^{85}Se	^{85}Br	^{85m}Kr	^{85}Kr	^{85}Rb
1.000																			
0.958	1.000																		
0.578	0.603	1.000																	
0.577	0.602	0.998	1.000																
0.000	0.000	0.000	0.000	1.000															
0.000	0.000	0.000	0.000	0.237	1.000														
0.041	0.000	0.000	0.000	0.225	0.948	1.000													
0.416	0.396	0.000	0.000	0.197	0.829	0.875	1.000												
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000											
0.417	0.397	0.002	0.000	0.197	0.829	0.875	1.000	0.000	1.000										
0.432	0.413	0.027	0.026	0.197	0.829	0.875	1.000	0.000	1.000	1.000									
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000								
0.000	0.000	0.000	0.000	0.762	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000							
0.000	0.000	0.000	0.000	0.764	0.052	0.000	0.000	0.000	0.000	0.000	0.000	0.985	1.000						
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000					
0.005	0.000	0.000	0.000	0.338	0.139	0.124	0.000	0.000	0.000	0.000	0.000	0.400	0.406	0.000	1.000				
0.005	0.000	0.000	0.000	0.338	0.139	0.124	0.000	0.000	0.000	0.000	0.000	0.400	0.406	0.000	1.000	1.000			
0.005	0.000	0.000	0.000	0.337	0.139	0.124	0.000	0.000	0.000	0.000	0.000	0.399	0.405	0.000	0.998	0.998	1.000		
0.001	0.000	0.000	0.000	0.072	0.030	0.026	0.000	0.000	0.000	0.000	0.000	0.086	0.087	0.000	0.215	0.215	0.214	1.000	
0.005	0.000	0.000	0.000	0.338	0.139	0.124	0.000	0.000	0.000	0.000	0.000	0.400	0.406	0.000	1.000	1.000	1.000	1.000	1.000

$$\begin{pmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \dots \\ b_{01} & 1 & 0 & \dots \\ b_{12}b_{01} & b_{12} & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} I_0 \\ I_1 \\ I_2 \\ \vdots \end{pmatrix},$$

Typical structure for beta- decay

Matrix elements due to delayed neutron beta- decay

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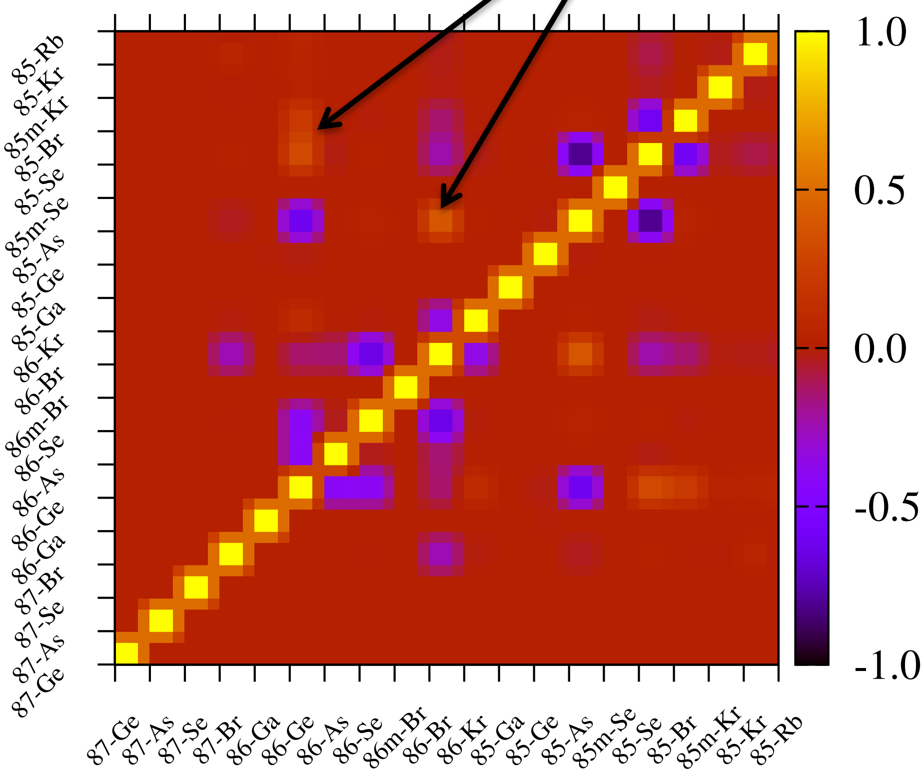
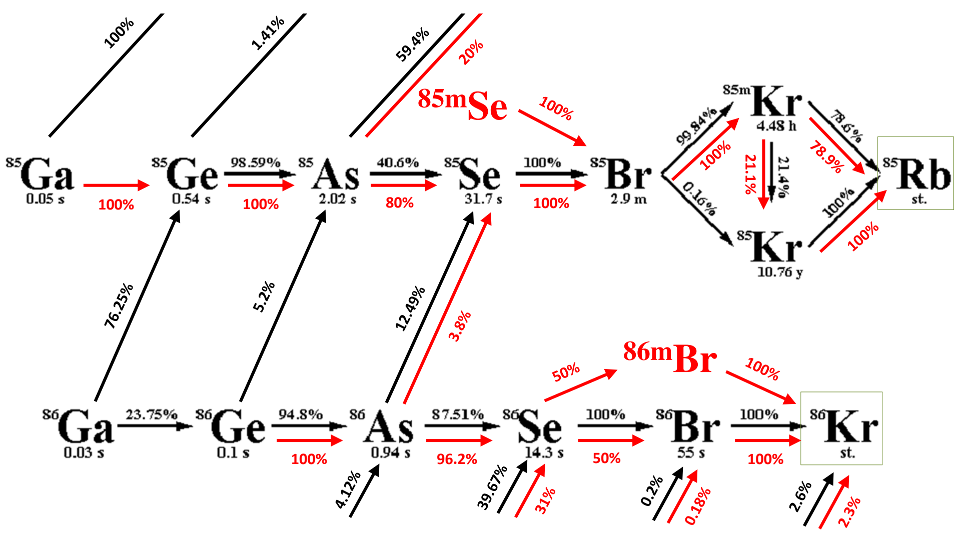
Results : krypton and xenon (Covariance data)

- **Strong negative correlations**
- **Relative strong positive correlations (delayed-neutrons)**



Decay scheme



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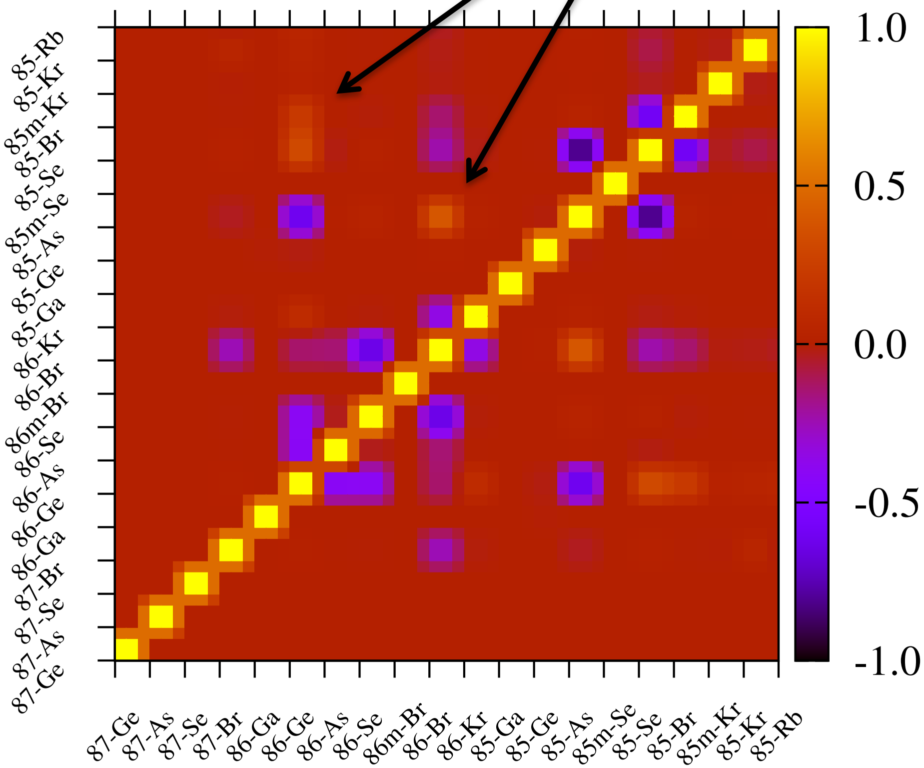

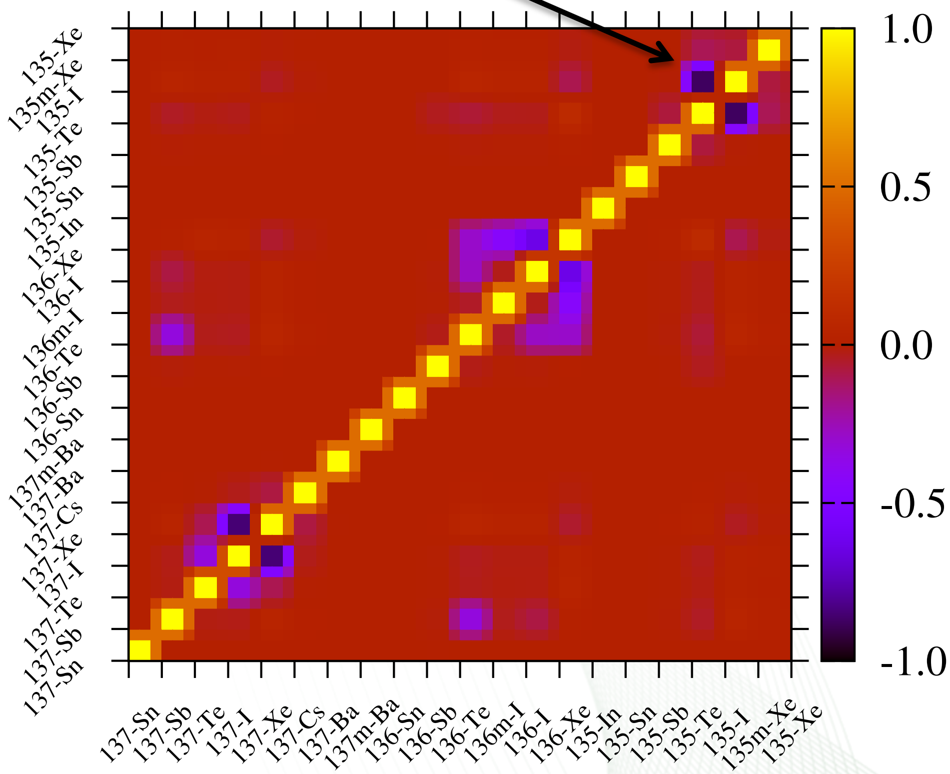

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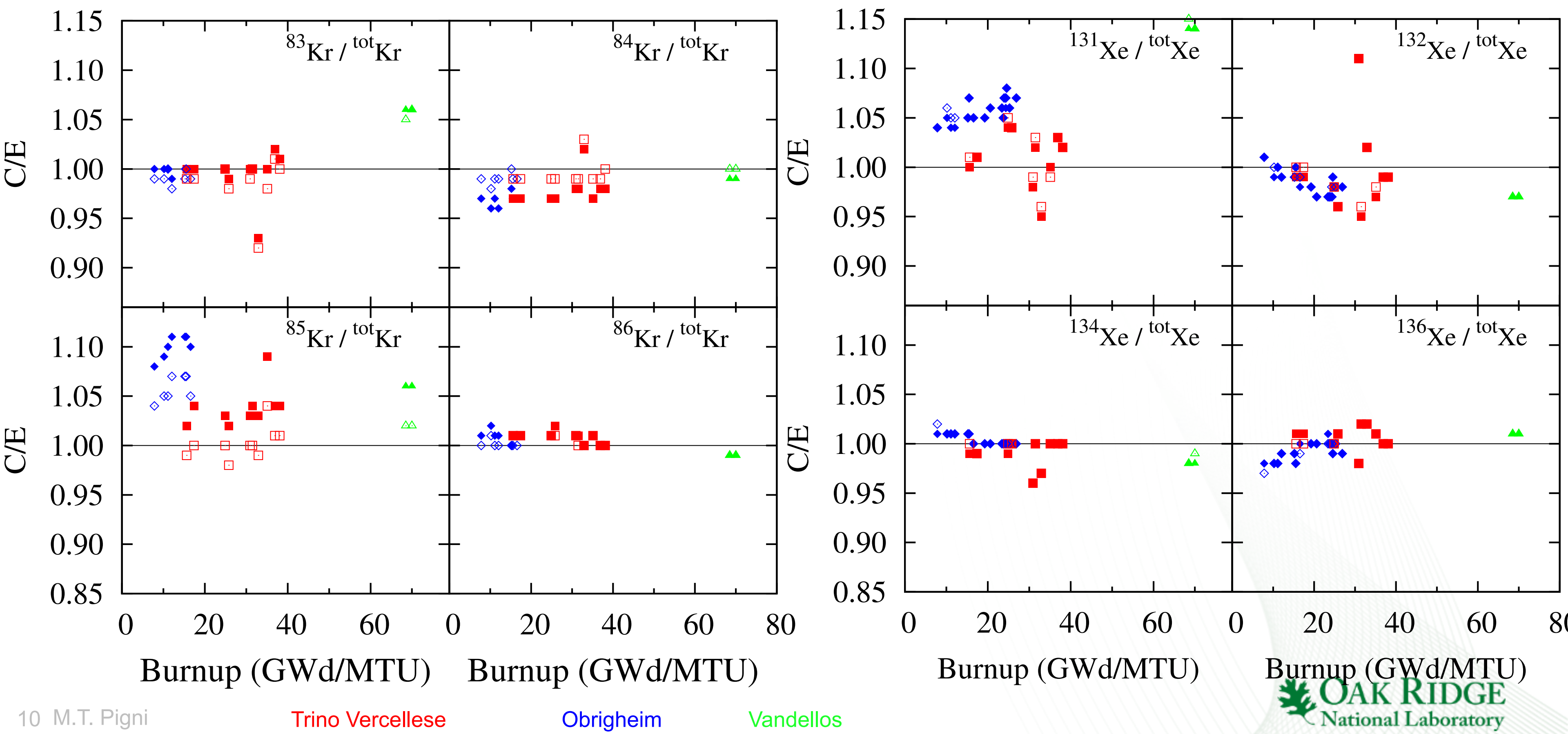
Results : Krypton and Xenon (New FPY Data vs Experiments)

ENDF/B-VII.1 library (full symbols, i.e., ◆, ■, ▲)

New ind. FPY library (empty symbols, i.e., ◇, □, △)



Summary / Conclusions

- **Results :**
  - In ENDF FPY sub-library there are two issues
    - Uncertainties too large for ind. FPY. They can not be used in applications
    - Consistency between decay and FPY sub-libraries
  - We generated complete covariance files for ind. FPY on ^{235}U(thr, 500keV,14MeV), ^{238}U(500kev), ^{239,241}Pu(thr)
  - We generated FPY data that improved agreement with experimental data for noble gases – krypton and xenon.
- **Future work :**
  - In the Bayesian method the model to obtain cumulative FPY was basically the decay scheme. An advanced (microscopic) fission model to generate ind. FPY would improve the prior information (P_0).
  - Improved Bayesian update keeping into account systematics of isobaric chains

Acknowledgments

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