Report on Status of SG39

WPEC/SG39

May, 2016

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Idaho National Laboratory

- Title: “Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files”
- Goals, Mandate, Working Method:
  - Mandate for this WPEC subgroup is to provide criteria and practical approaches to use effectively the results of sensitivity analyses and cross section adjustments for feedback to evaluators and differential measurement experimentalists in order to improve the knowledge of neutron cross sections, uncertainties, and correlations to be used in a wide range of applications.
  - Review issues and summarize findings on methodologies used to provide feedback to evaluated data files (e.g. reactor physics experiment accuracies, adjustment methodologies etc.).
  - Select and define test cases for application.
  - Based on obtained results, recommend a general methodology and practices for providing feedback to evaluators both on nuclear data and on associated covariance data, based on specific examples.
  - Actual feedback will be provided to evaluation projects (e.g. CIELO initiative) on the specific examples indicated in the previous point.

Current Activities

- **Finalize several deliverables.**
- **Analyzing and using new experiments of elemental and separation of effects type: PROTEUS, FCA-IX, SEG, ASPIS-88, SNEAK, MANTRA.**
- **Developing new adjustment strategies for both: coping with the compensation issue and make more compatible with current calculational tools (continuous energy).**
- **Providing industry support for quantification and reduction of uncertainty using data assimilation.**

Finalize deliverables

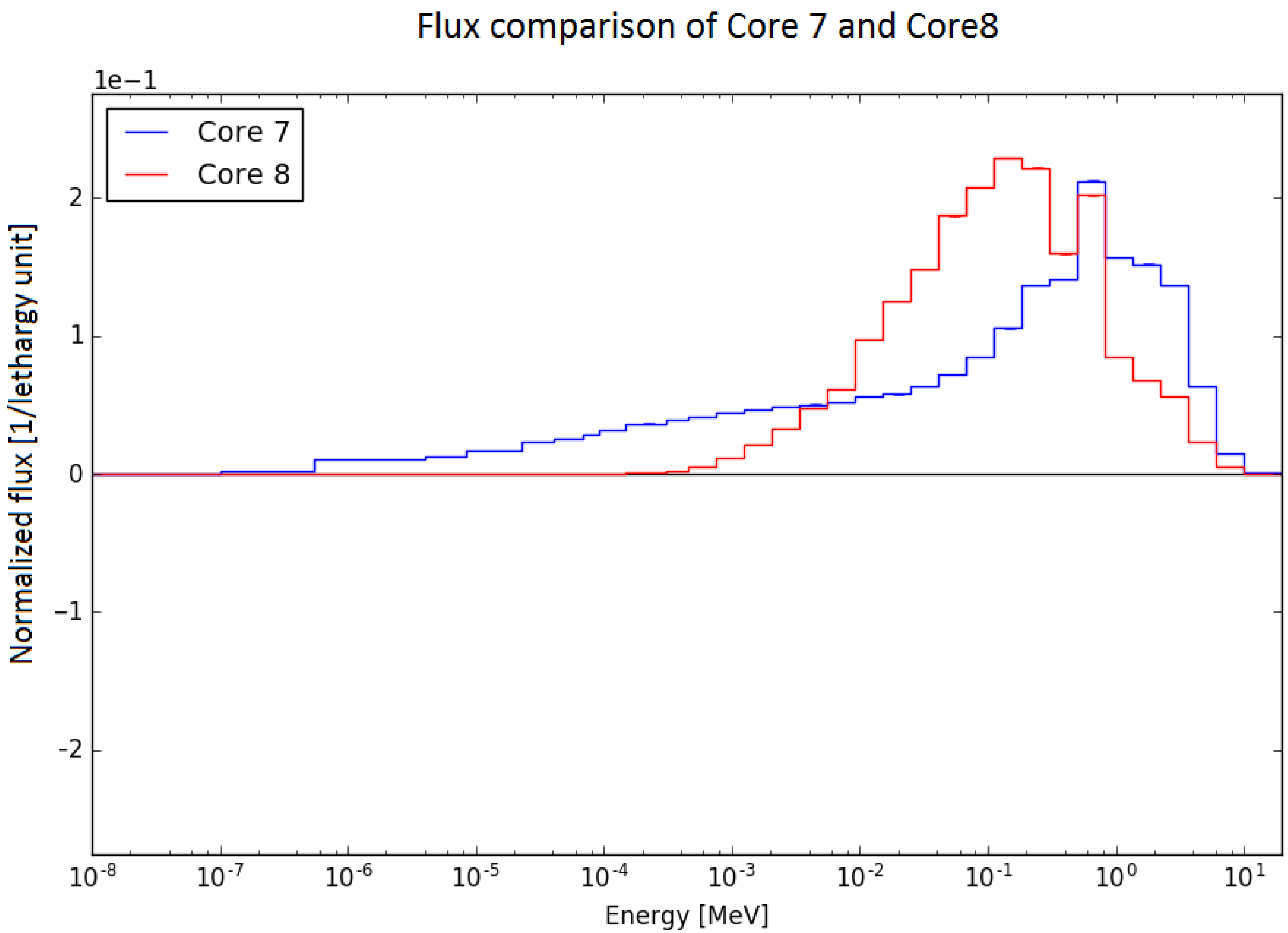
- The intermediate report, titled "Methodologies and Covariance Data", has been finalized and sent for publication (out very soon). It contains the covariance data assessment (M. Ishikawa) and the development of methodology for coping with the problem of compensation (key topic).
- Sensitivity coefficients deliverable, MC vs deterministic and other issues, is still pending.
- Produce report on the status of uncertainties of Am-241. Initiate by criticality safety problem for space application. Waiting for final input from industry.

Last year we did point out the need to use *new integral experiments for separate physics effects* as a basic requirement to avoid the compensations often associated to the use of global parameters as keff.

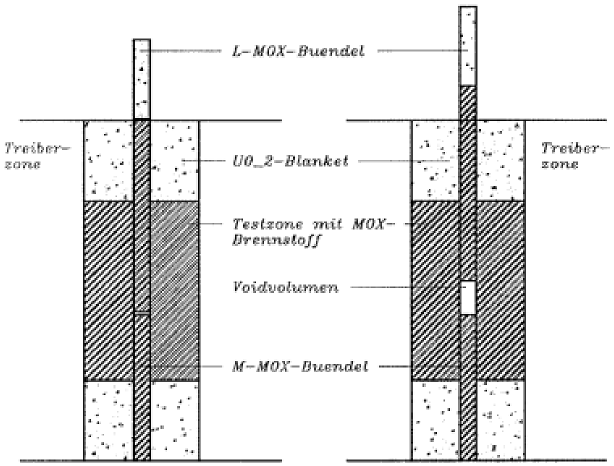
- **Most of the experiments suggested at the time are now available as well as the associated sensitivity coefficients:**

- **PROTEUS (link between epithermal and fast energy range: k- infinity, void coefficient, reaction rate ratios): U-238, Pu isotopes**
- **Beff experiments (new inelastic information, but need delayed nubar uncertainty). U-238, Pu-239, U-235**
- **Variable adjoint experiments (SEG) to separate inelastic from absorption effects.**
- **Selected neutron propagation experiments (inelastic, elastic). Mostly Fe, also Na-23**
- **FCA experiments, related to actinide data (MA and higher Pu isotopes)**

FDWR-II - Spectrum Comparison



FDWR-II – Measurement types

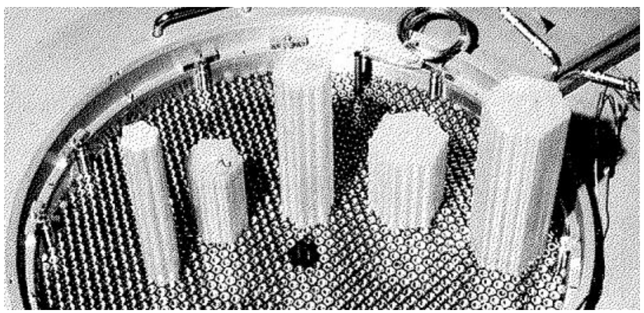


- K∞ measurements

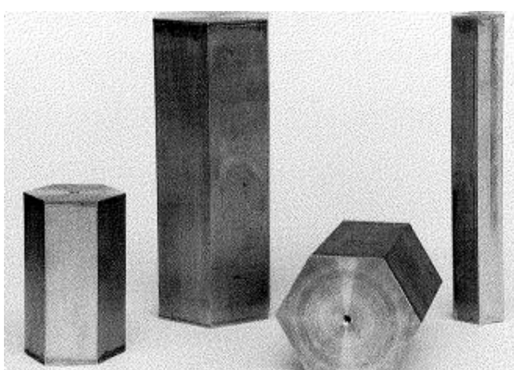
$$k_\infty = 1 + B^2 \cdot M^2$$

$$\frac{\rho_Z}{\rho_S}\frac{S}{R_f} = \bar{\nu}\frac{\overline{\Phi^+}^X}{\overline{\Phi^+}^S}\left(1 - \frac{1}{k+}\right)$$

  - Using axial and radial bucklings
  - Using compensation methods with auto-rod and a ^{252}Cf source

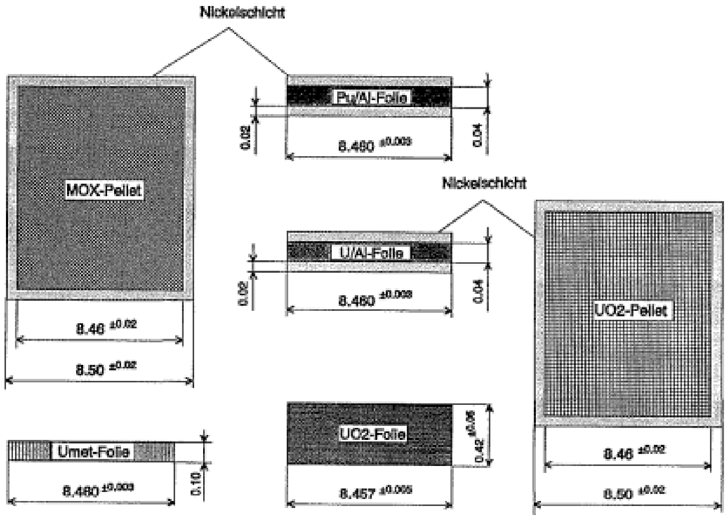


- Reactivity effects
  - Void volume



Absorber	Form	Durchmesser	Cladding	Bemerkung
B_4C(nat)	Pellet	7.473	ja	Referenzabsorber
B_4C(nat)	Pulver	7.430	ja	
B_4C(93%) ^{10}B	Pellet	7.430	ja	
Ag15In5Cd	Legierung	8.830	nein	
Hafnium	Metall	8.350	ja	
Gd_2O_3	Pellet	8.310	ja	
Sm_2O_3	Pellet	7.000	ja	
Tantal	Metall	8.290	ja	
Eu_2O_3	Pellet	8.243	ja	
Zircaloy-2	Legierung	8.300	nein	Strukturmaterial
Stahl	Metall	8.240	nein	Strukturmaterial

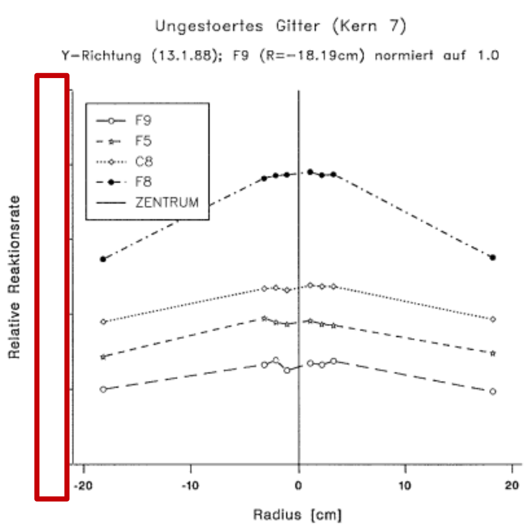
FDWR-II – Measurement types

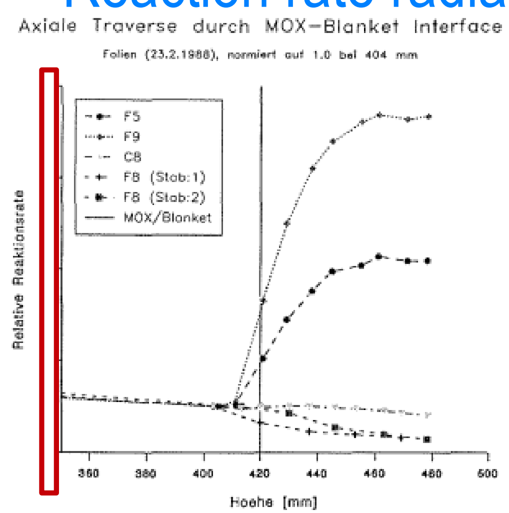


Spectral index measurements (core 7)

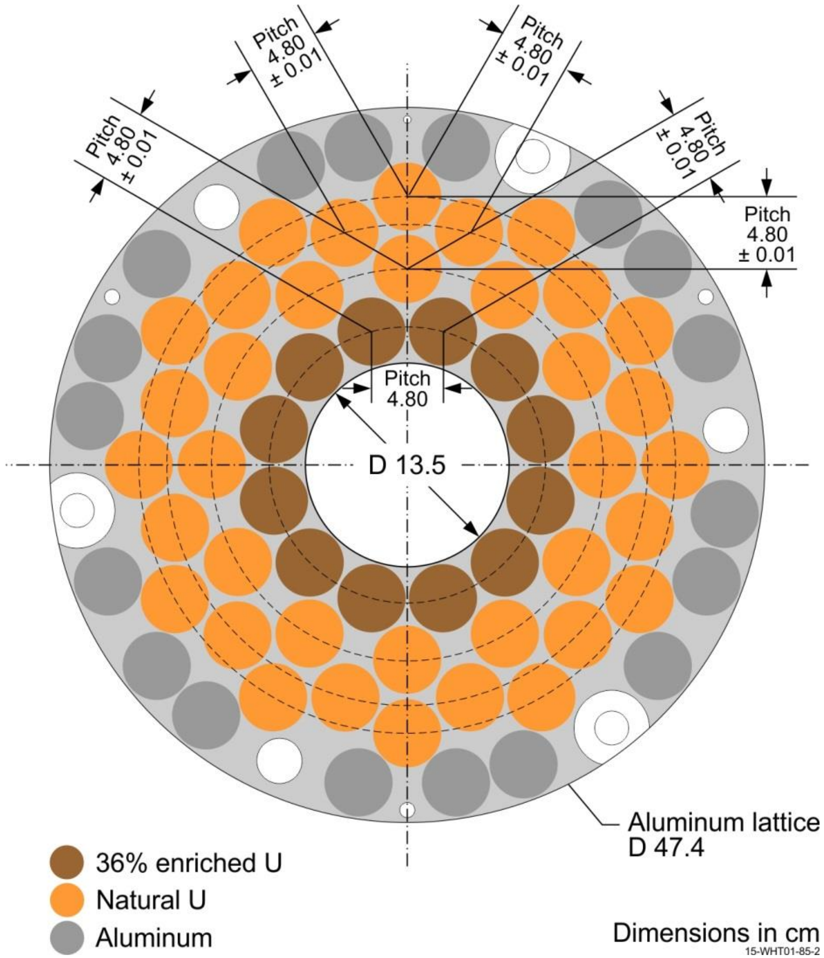
- F5/F9 ~0.91 F1/F9 ~ 1.68
- F8/F9 ~1.14e-2 C2/F9 ~ 1.12
- C8/F9 ~7.8e-2
- Typical uncertainties
  F5: 1.8%, F8: 1.9%, F9:1.5%, C8: 1.8%

Reaction rate radial and axial traverses



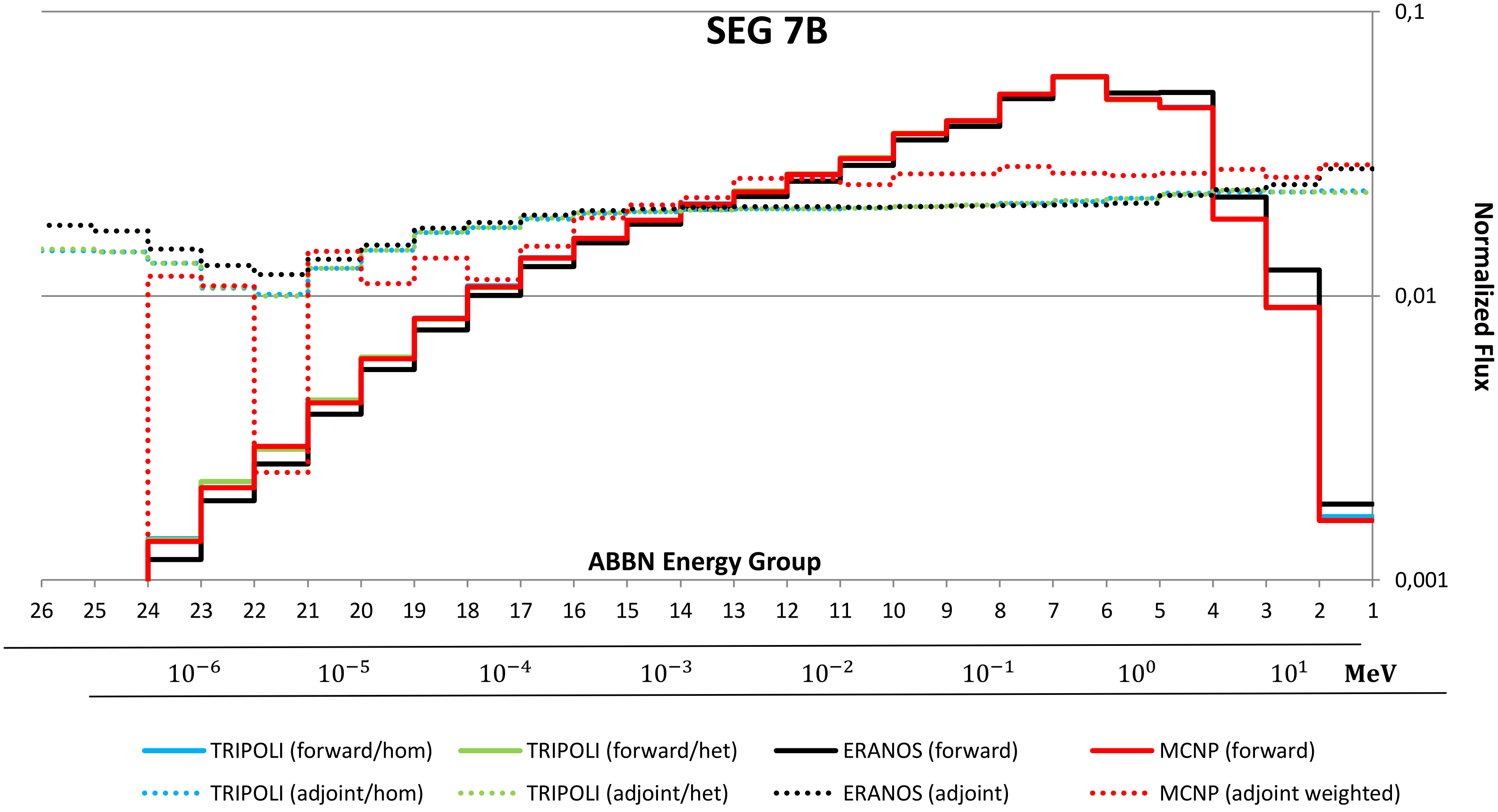


RRR/SEG Fast-Thermal Coupled Facility

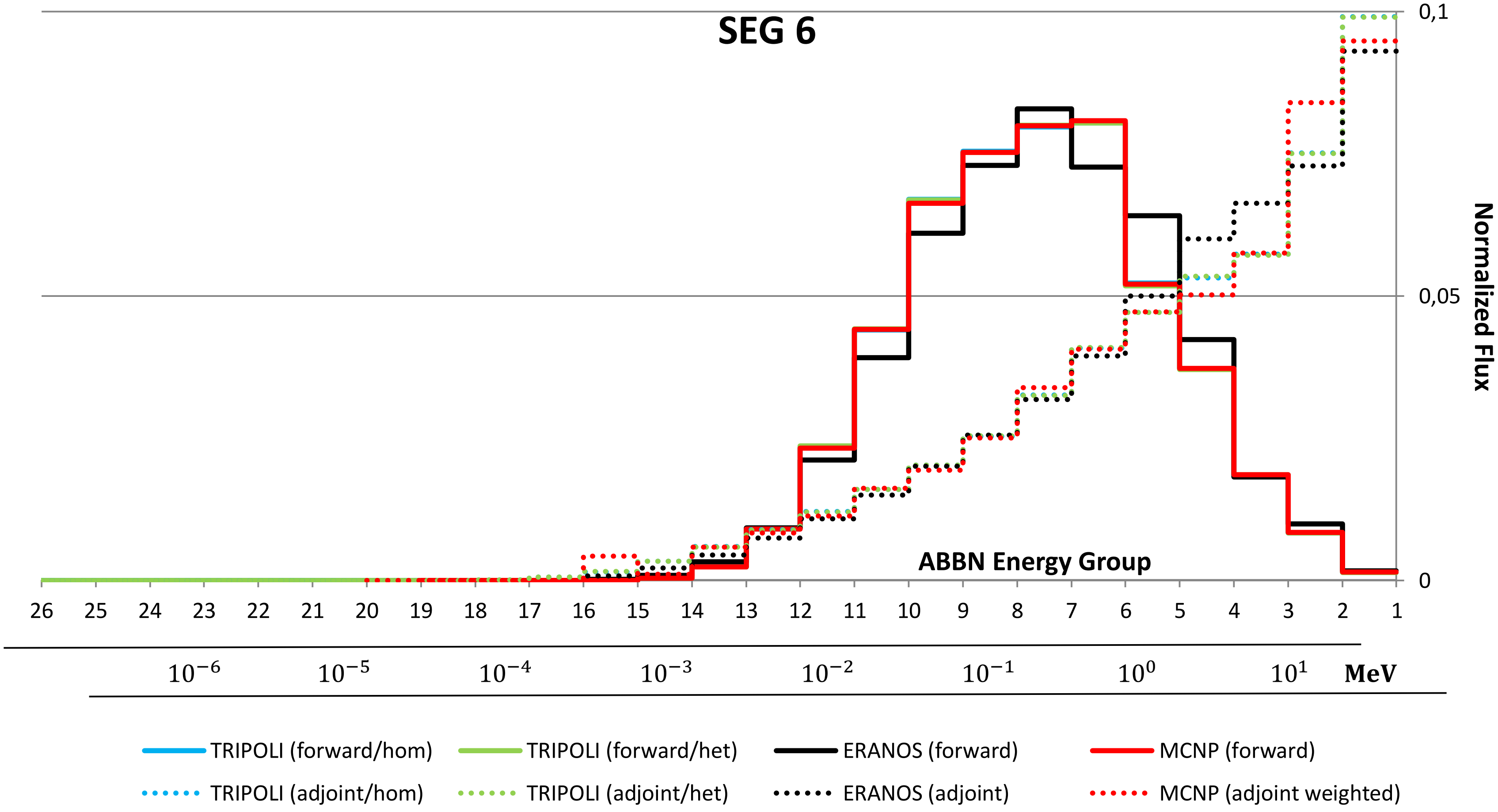


- SEG 6 lattice
  - Radial arrangement of 4 rings each having 12 channels
  - Inner ring: 36% enriched U
  - Outer 3 rings: natural U
  - Inner absorption zone: B_4C
  - Experimental channel is either 5.0 or 1.2 cm in diameter
  - Natural U converter surrounded by annular driver fuel

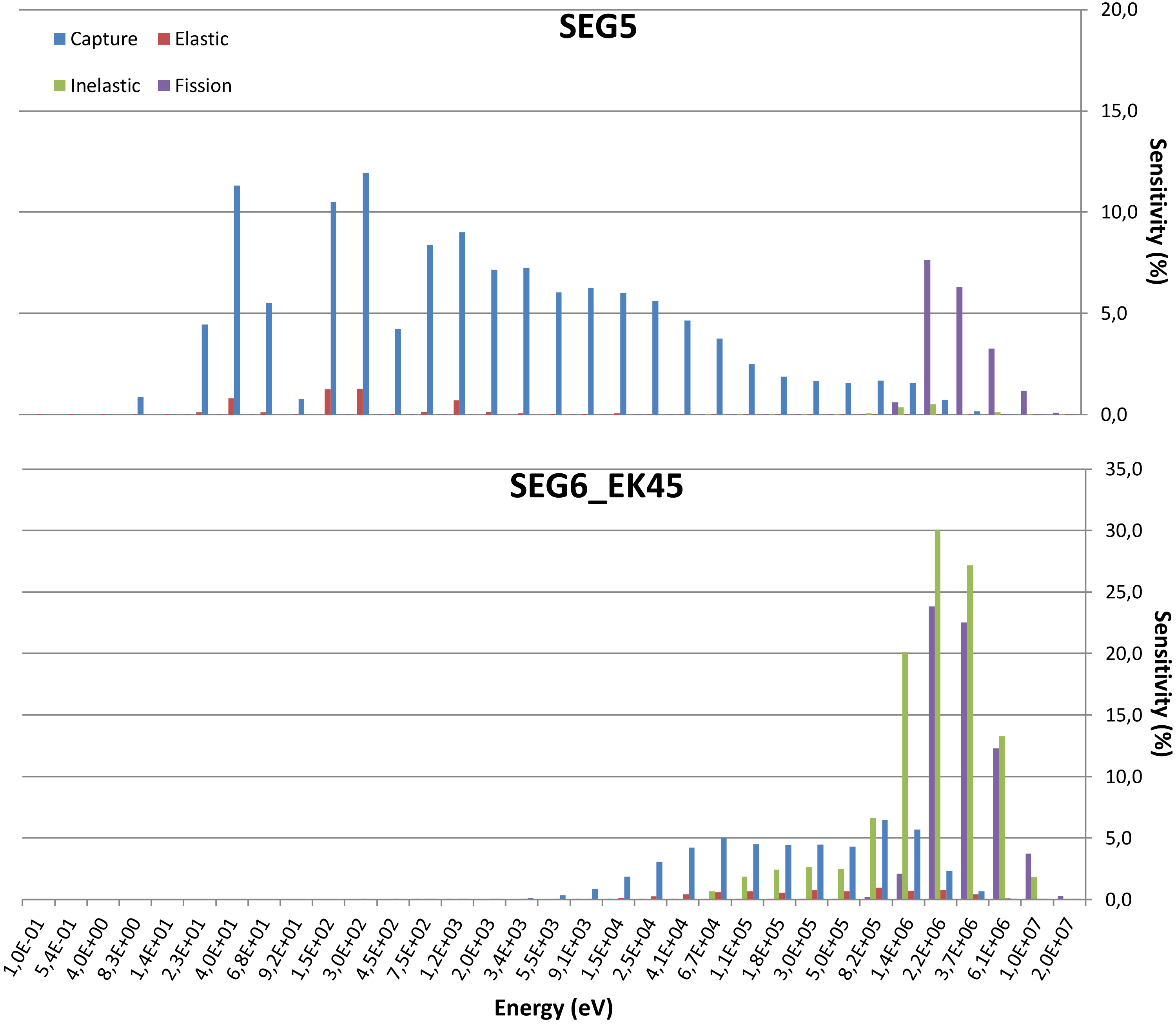
Forward and Adjoint Flux Spectrums



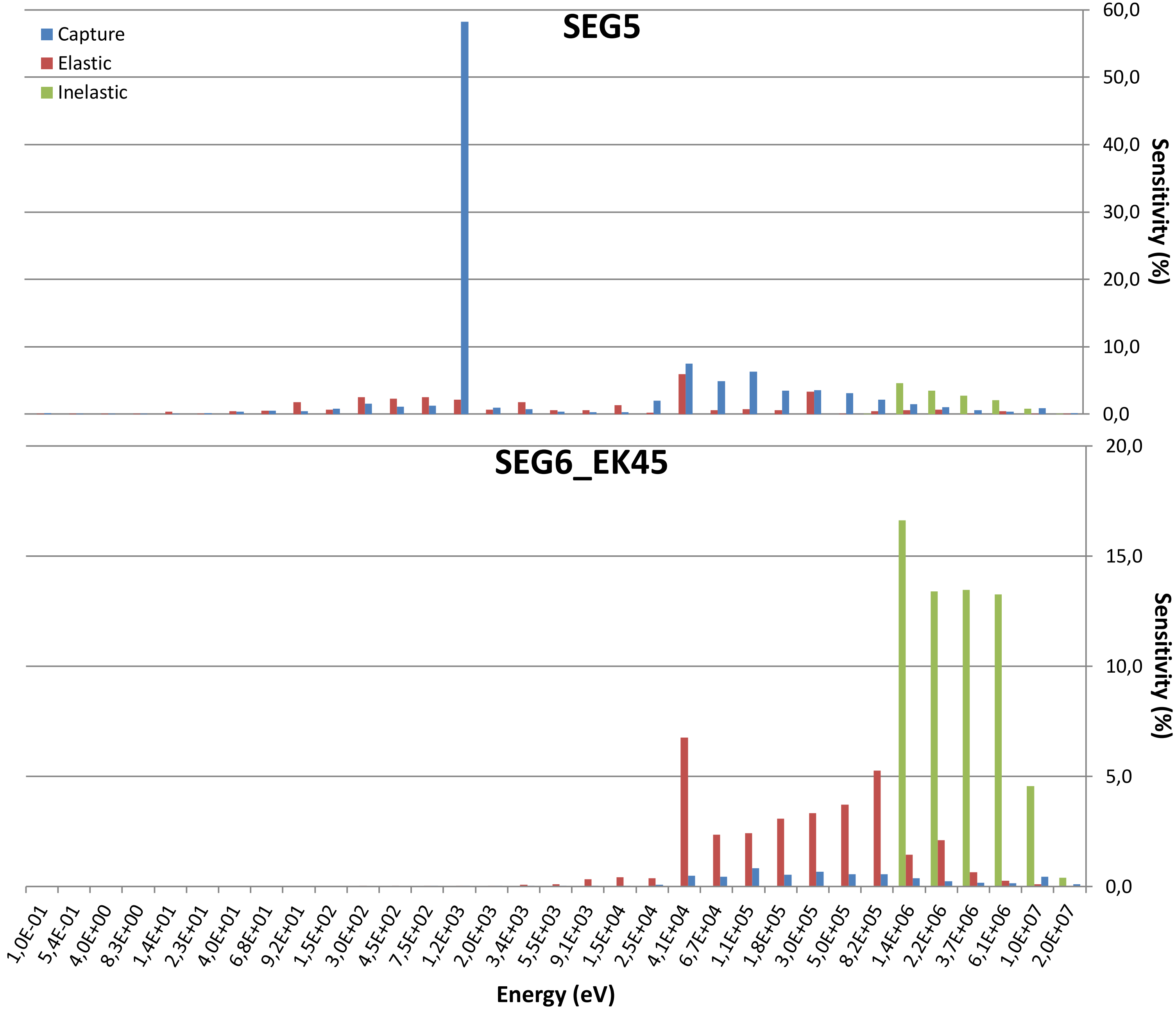
Forward and Adjoint Flux Spectrums



U-238 Sensitivities (JEFF-3.2/TRIPOLI)



Fe-56 Sensitivities (JEFF-3.2/TRIPOLI)



ASPIS IRON-88

Au, Rh, In, S and Al activation foils installed in 7.4-mm air gaps.

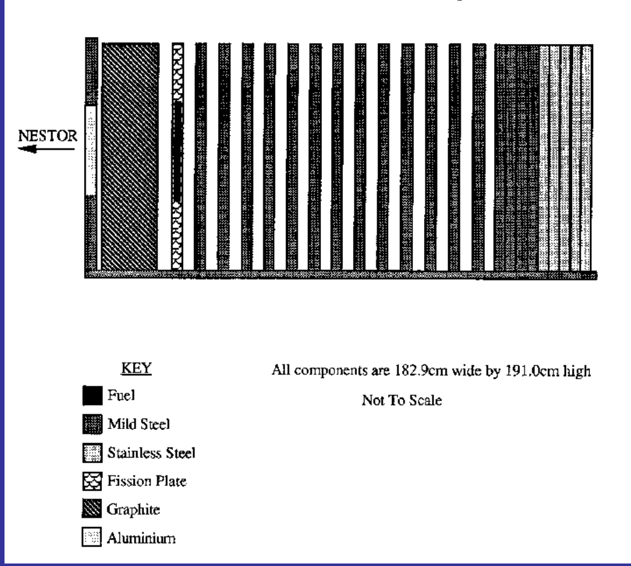


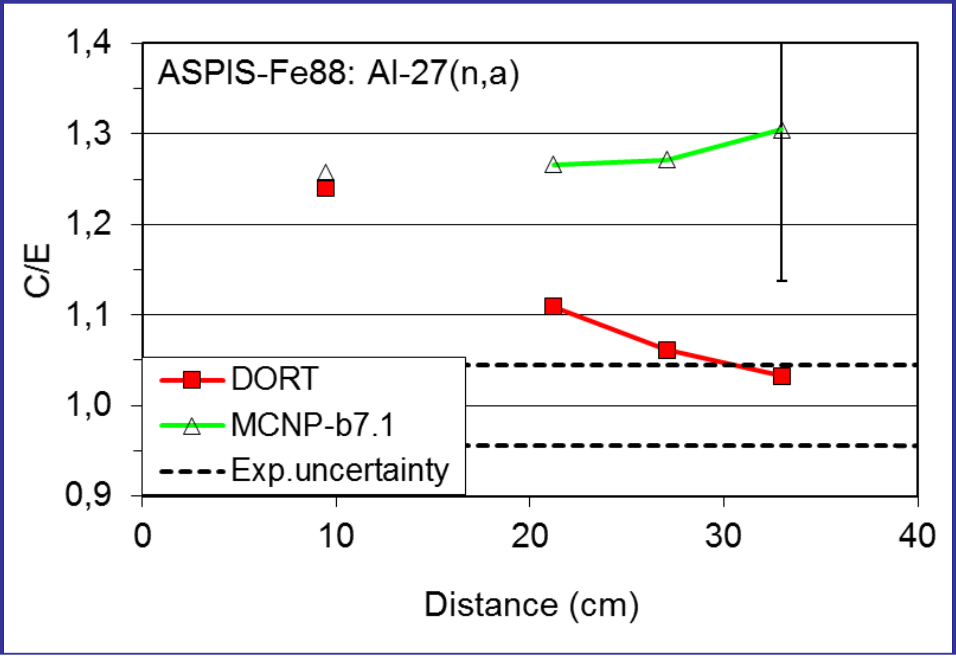
Figure 1 Schematic side elevation of the shield in the iron 88 single material benchmark experiment

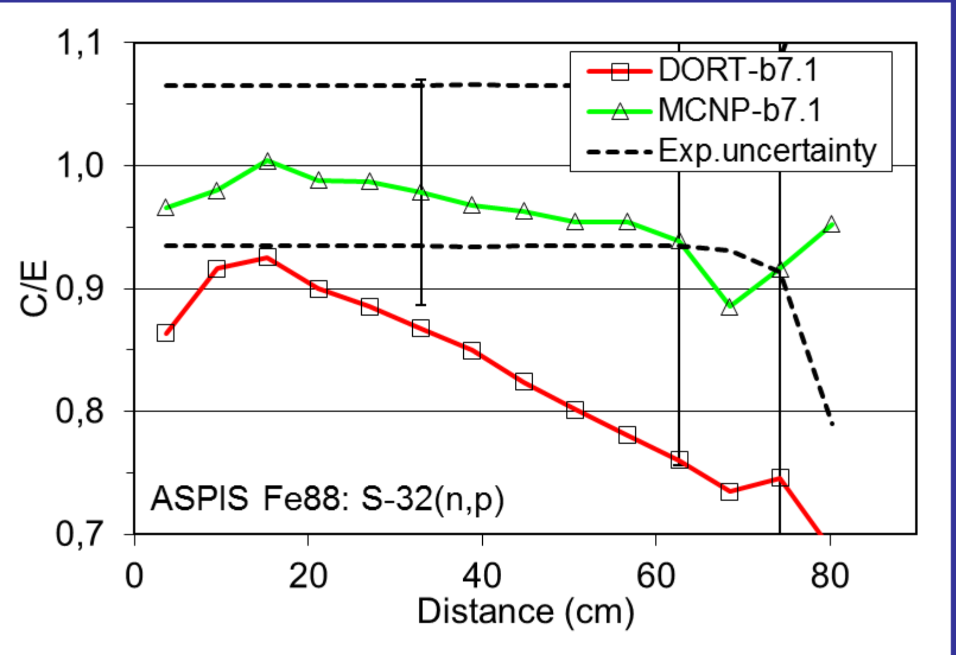
Detector	Diameter (mm)	Thickness (mm)	Typical Mass (g)	Cadmium Cover (inches)	Counting System	Systematic Absolute Calibration (2σ uncertainty)
Au197(n,gamma)	12.7	0.05	0.12 -0.13	50/1000	NaI	0.9%
Rh103(n,n')	12.7	0.015	0.20	-	NaI	3.0%
In115(n,n')	38	1.63	12.79	-	GeLi detector	1.9%
S32(n,p) Pressed Pellet	38.1	2.41	5	-	Plastic Scintillator	5.0%
S32(n,p) Cast Pellet	51	5.6	22	-	Plastic Scintillator	5.0%
Al27(n,alpha)	50	3.1	16.72	-	Ge detector	2.2%

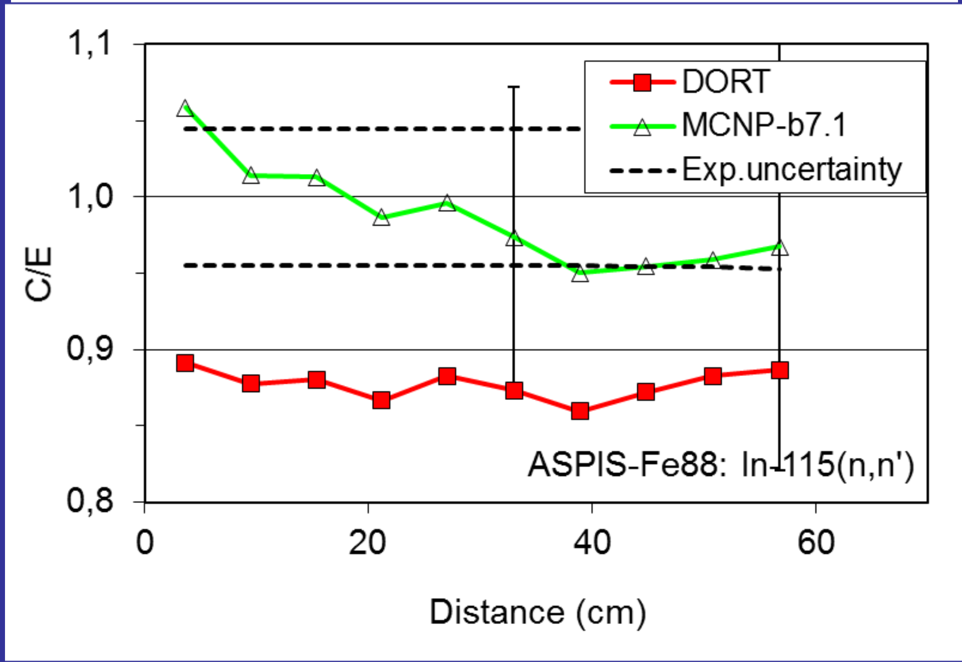
Transport & S/U analysis

C/E comparison

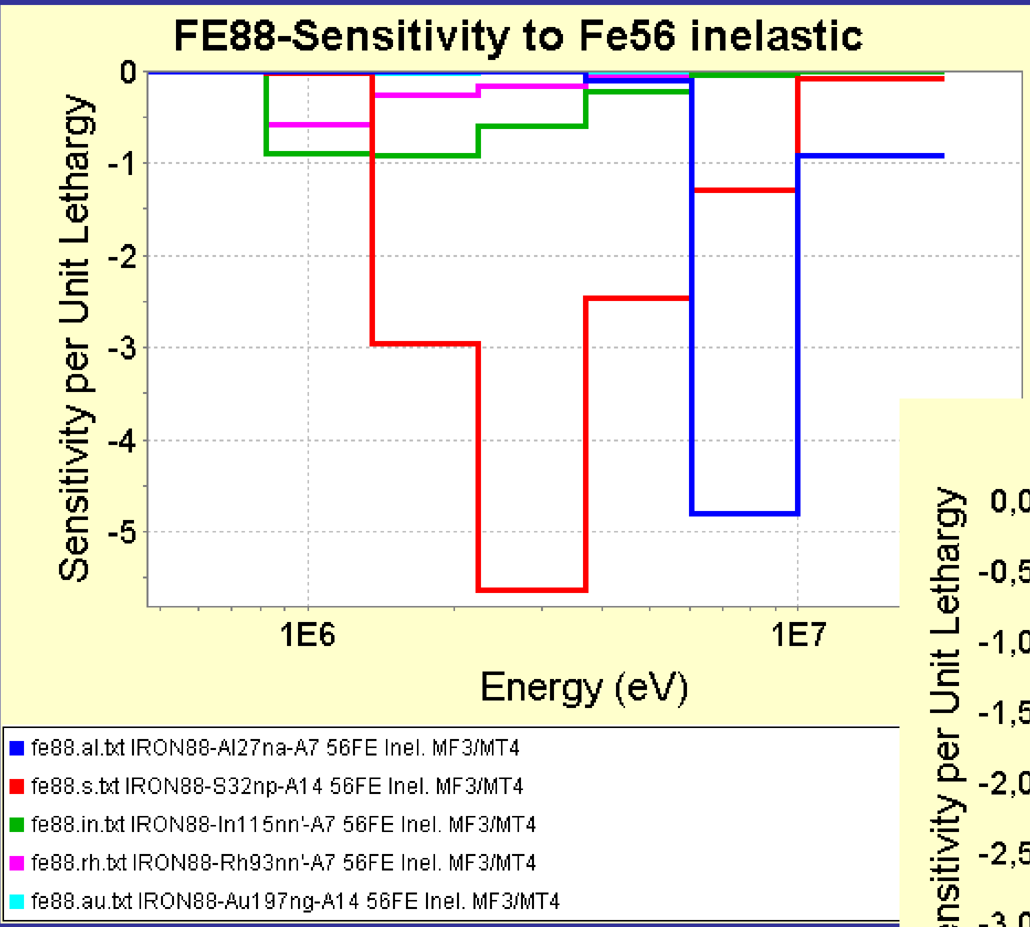
- **MCNP** using ENDF/B-VII.1 & CIELLO xs
- **DORT/SUSD3D** simplified 2D model using ECCO 33-group ENDF/B-VII.1 xs. Used for xs sensitivity/uncertainty analysis.
- **ΔC >> ΔE !!!!!**

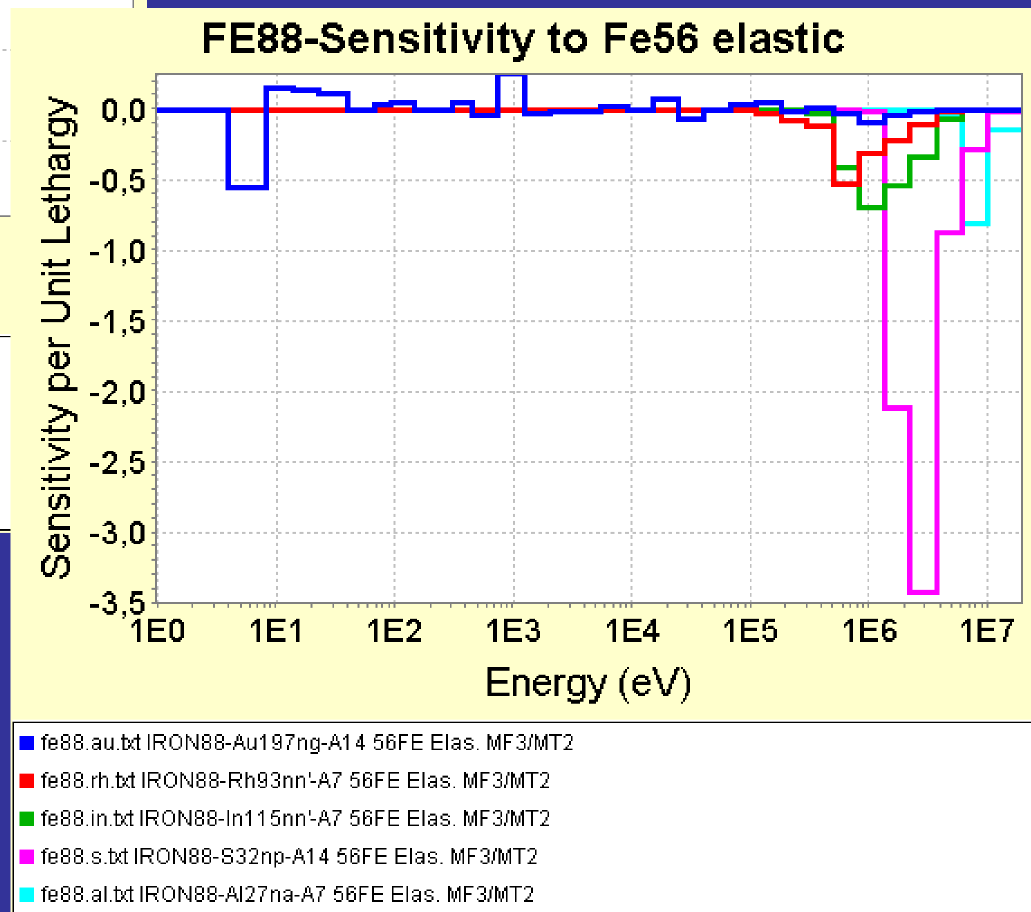




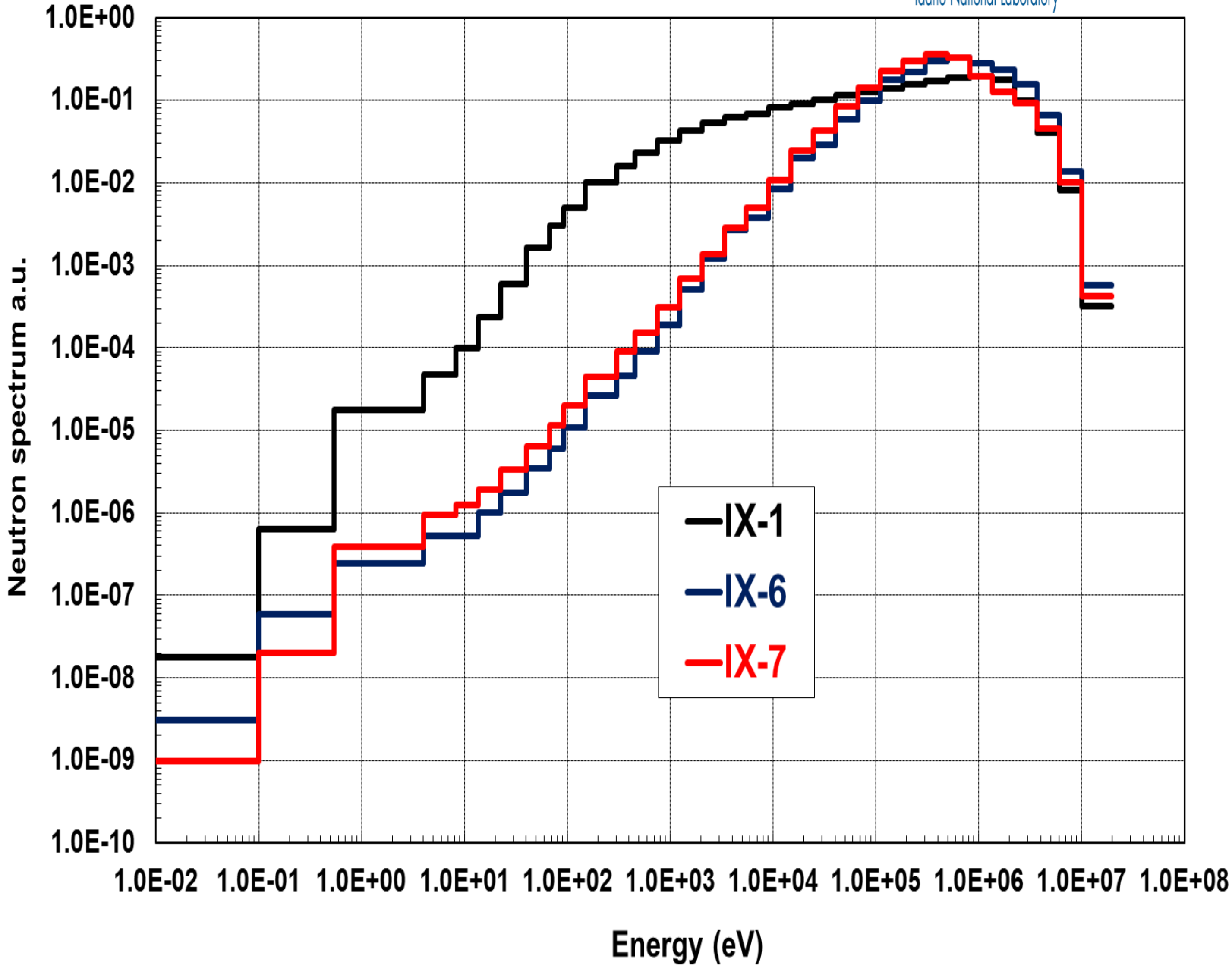


Sensitivity (SUSD3D/DORT)

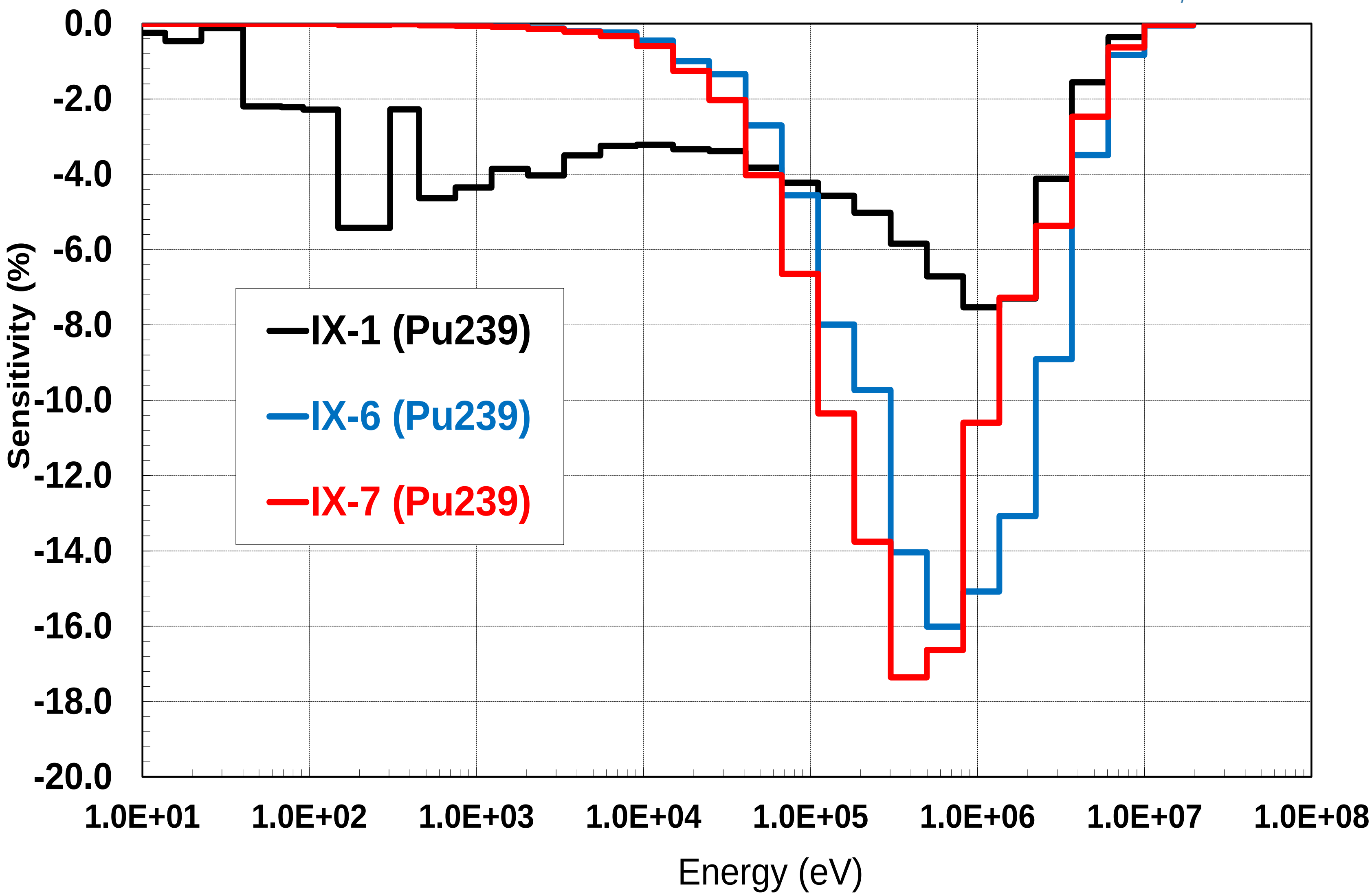




Neutron Spectra in the Reactor Center

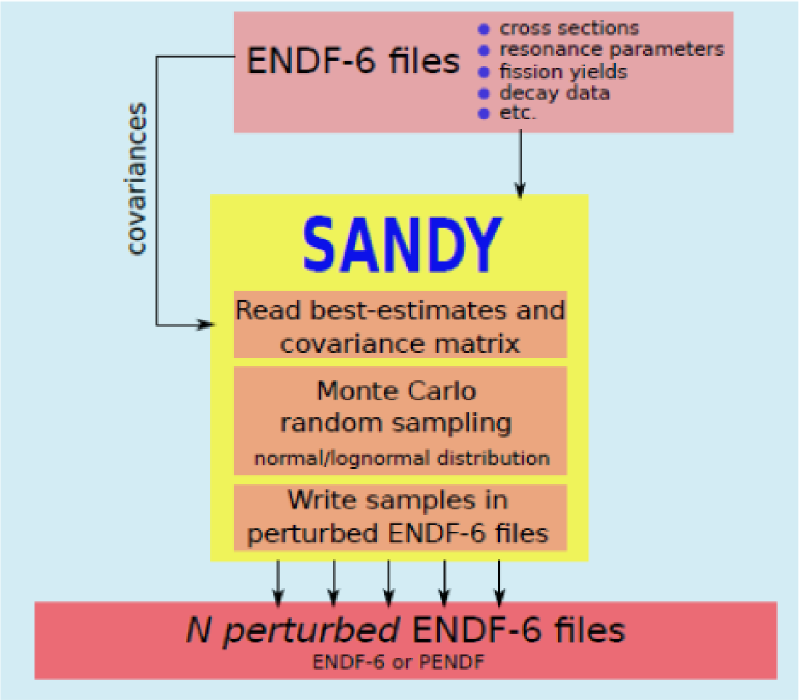


Sensitivity of ^{239}Pu σ_{fiss} (direct effect on spectrum index denominator)



What is SANDY?

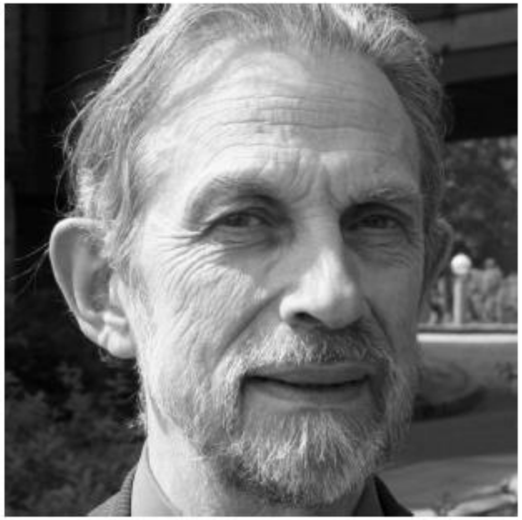
- Numerical tool for nuclear data uncertainty quantification
- Based on Monte Carlo sampling
  - Input parameters random samples are generate according to best-estimate data and covariances
  - Normal or LogNormal multivariate PDF
  - Not dependent on the model and on the model solver (black box)
  - No linerarity assumption
  - Accuracy related to the number of samples
- Compatible with ENDF-6 format
- Pointwise parameters (no multi-group assumption)
- Flexibility: many libraries, many codes (MCNP)
- SANDY was tested for linear models against TSUNAMI and perturbation theory obtaining analogous results.



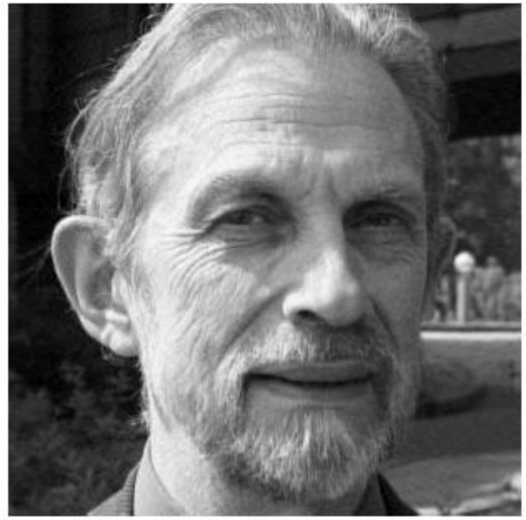
k_{eff} uncertainty quantification with SANDY

Isotope	uncert. k_{eff} (pcm) (ENDF/B-VII.1)	Reaction	Variance decomposition	uncert. K_{eff} (pcm) (JENDL-4.0)
Bi-209 (XS)	201 ± 34	(n,elastic)	55 ± 17	-
		(n,inelastic)	133 ± 38	-
		(n,gamma)	143 ± 41	-
U-235 (XS)	5511 ± 1233	(n,elastic)	35 ± 11	-
		(n,inelastic)	273 ± 86	-
		(n,fission)	264 ± 83	-
		(n,gamma)	5477 ± 1734	-
U-238 (XS)	1161 ± 183	(n,elastic)	49 ± 16	-
		(n,inelastic)	1065± 337	-
		(n,fission)	53± 19	-
		(n,gamma)	326 ± 103	-
U-235 (ν_p)	179 ± 57	-	-	367± 116
U-238 (ν_p)	189± 60	-	-	99± 31

Singular Value Decomposition



Original
image

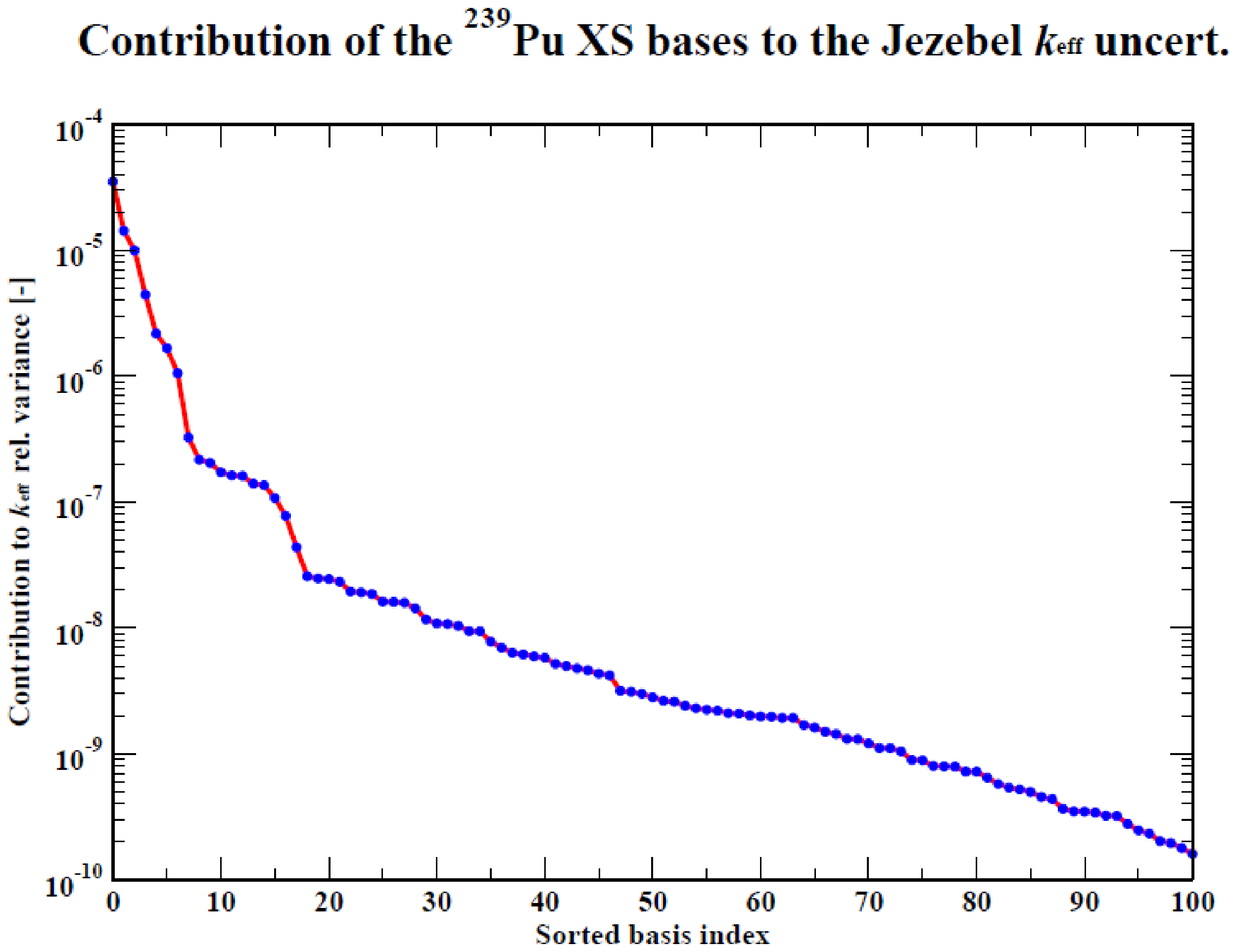


SVD/POD
80 basis functions

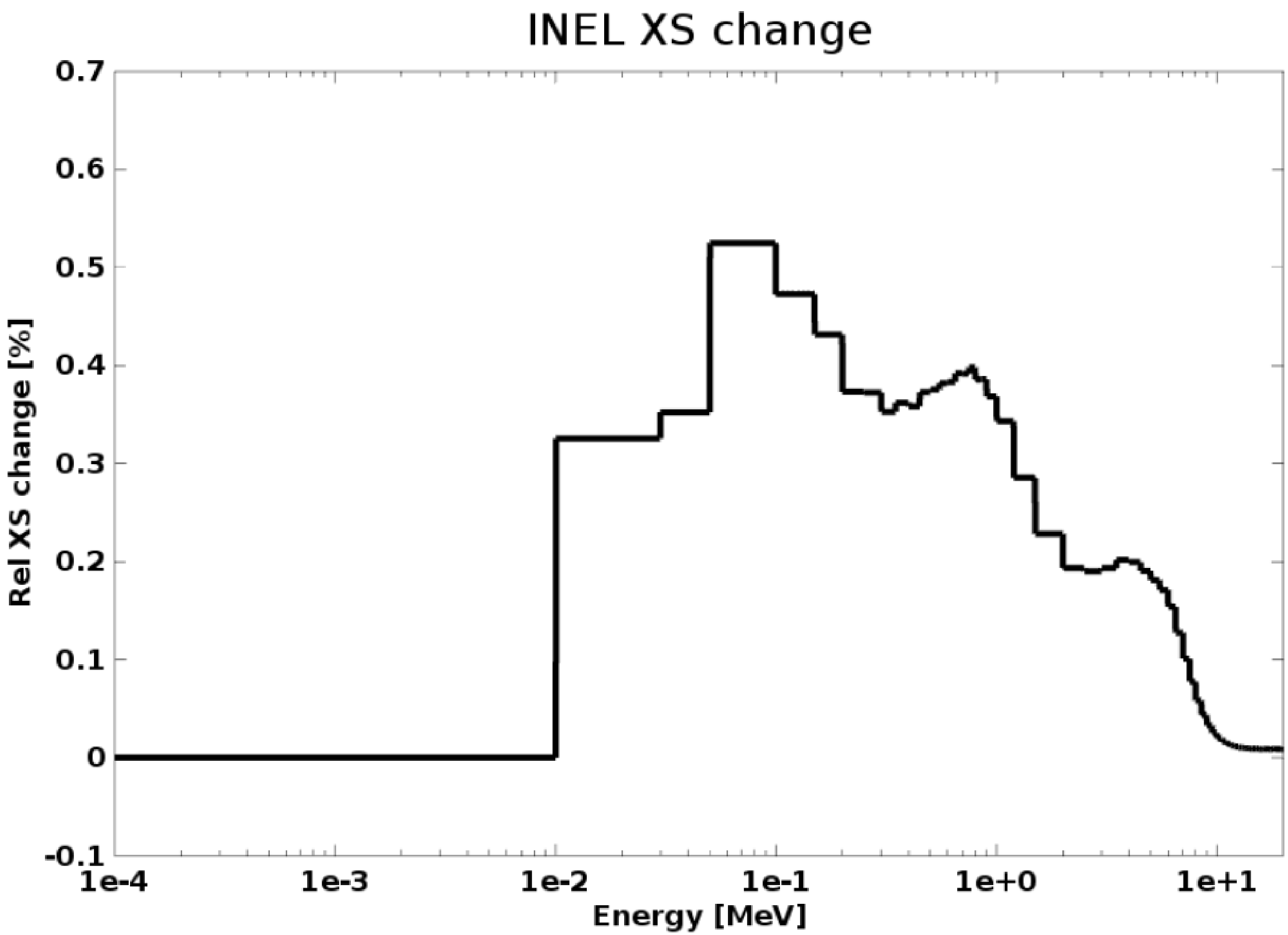
Multi-group
80 energy groups

```
A=imread("massimo.png"); [A, map]=gray2ind(A,255);
[U, S, V]=svd(A);
A_SVD_80 = U(:,1:80) * S(1:80,1:i) * V(:,1:80)';
imwrite(A_SVD_80, gray(255), "massimo_80.png");
```

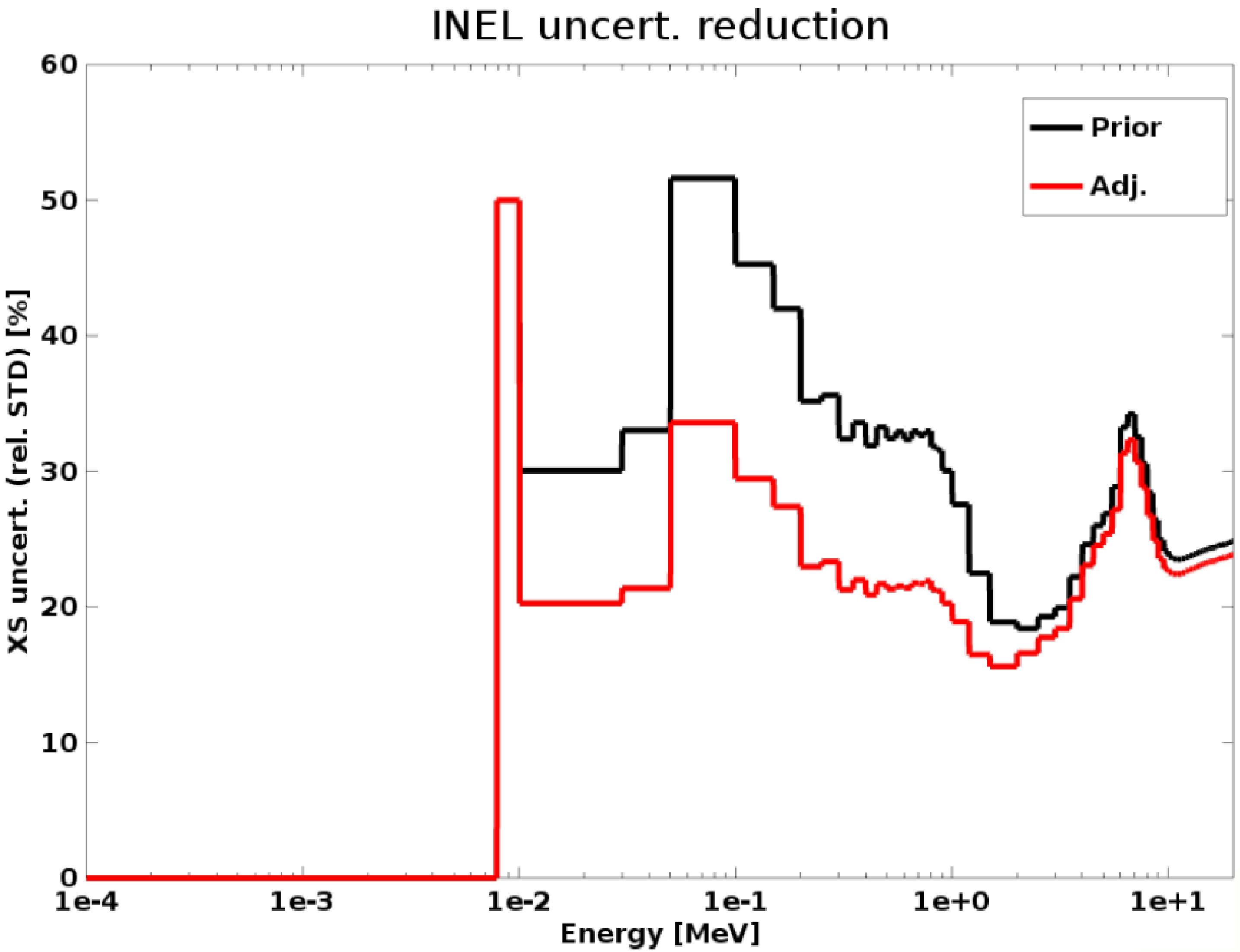
Adjustment via XGPT: first attempt



Adjustment of the inelastic XS



Small reduction of the inelastic uncertainty



Development of new adjustment strategies

- **In order to cope with the key issue of compensation of effects new adjustment strategies are under development:**
  - **PIA (Progressive Incremental Adjustment)**
  - **REWIND (Ranking Experiments by Weighting for Improved Nuclear Data)**
- **An attempt has been made to combine the two methodologies**
- **The new methodology has been applied to the SG33 experiment list**

Application to the SG33 Experiments

- The methodology has been applied to the case of the 20 experiments of the SG33 exercise.
- Results are compared against the initial values (ENDF/B-VII.0 for cross sections and COMMARA 2.0 for standard deviations) and the results of the traditional (global) adjustments where all the experiments are considered at once.
- Results indicated:
  - In some cases there are differences on the central values of the cross sections.
  - Standard deviations tend to be systematically lower (except partially for one specific case) when the new methodology is applied.
  - One can expect a bigger impact if more experiments of elemental type are used (e. g. large ENDF/B-VII.0 adjustment).
  - The procedure is quite cumbersome (12 adjustments performed with several intermediate steps).

REWINDing PIA applied to SG33 experiments and 5 Isotopes: ^{23}Na, ^{56}Fe, ^{235}U, ^{238}U, ^{239}Pu

Experiment	Optimal weight %	Rank	Sharpe Ratio	C/E before adjust.	C/E after adjust.	Uncert. before adjust. %	Uncert. after adjust. %
JEZ_Pu239 F28/F25	67.4	1	0.61	0.9770	1.0025	3.75	0.59
JEZ_Pu239 F37/F25	0.0	3	0.39	0.9870	0.9963	2.38	0.42
JEZ_Pu239 F49/F25	0.0	3	-0.15	0.9753	0.9960	0.82	0.31
FLATTOP F28/F25	0.0	3	0.40	0.9822	0.9905	3.12	0.56
FLATTOP F37/F25	0.0	3	0.30	0.9956	1.0078	2.05	0.41
ZPR6/7 F28/F25	0.0	3	0.46	1.0045	1.0121	6.48	0.87
ZPR6/7 F49/F25	0.0	3	-2.07	0.9638	0.9786	0.84	0.41
ZPPR9 F28/F25	32.6	2	0.64	0.9710	0.9895	8.02	0.90
ZPPR9 F49/F25	0.0	3	-1.47	0.9808	0.9958	0.87	0.40
ZPR6/7 C28/F25	0.0	2	-0.78	1.0098	0.9985	1.51	0.51
ZPPR9 C28/F25	100.0	1	-0.29	1.0093	0.9999	1.55	0.51
JEZ_Pu239 KEFF	7.6	4	0.69	0.99986	1.00011	0.74	0.11
JEZ_Pu240 KEFF	0.0	5	0.59	0.99981	0.99999	0.73	0.13
FLATTOP KEFF	44.3	1	0.65	1.00097	1.00015	0.88	0.14
ZPR6/7 KEFF	0.0	5	0.77	1.00043	1.00038	1.00	0.09
ZPR6/7 PU40 KEFF	0.0	5	0.78	0.99937	0.99935	1.00	0.08
ZPPR9 KEFF	36.5	2	0.90	0.99922	1.00009	1.22	0.08
JOYO KEFF	11.7	3	0.79	0.99746	0.99991	0.90	0.14
ZPPR9 STEP3	0.0	2	-0.02	1.0192	1.0272	7.65	3.09
ZPPR9 STEP5	100.0	1	0.23	0.9732	0.9822	9.90	3.77

χ^2 Before Adjust: 0.90 After Adjust.: 0.14

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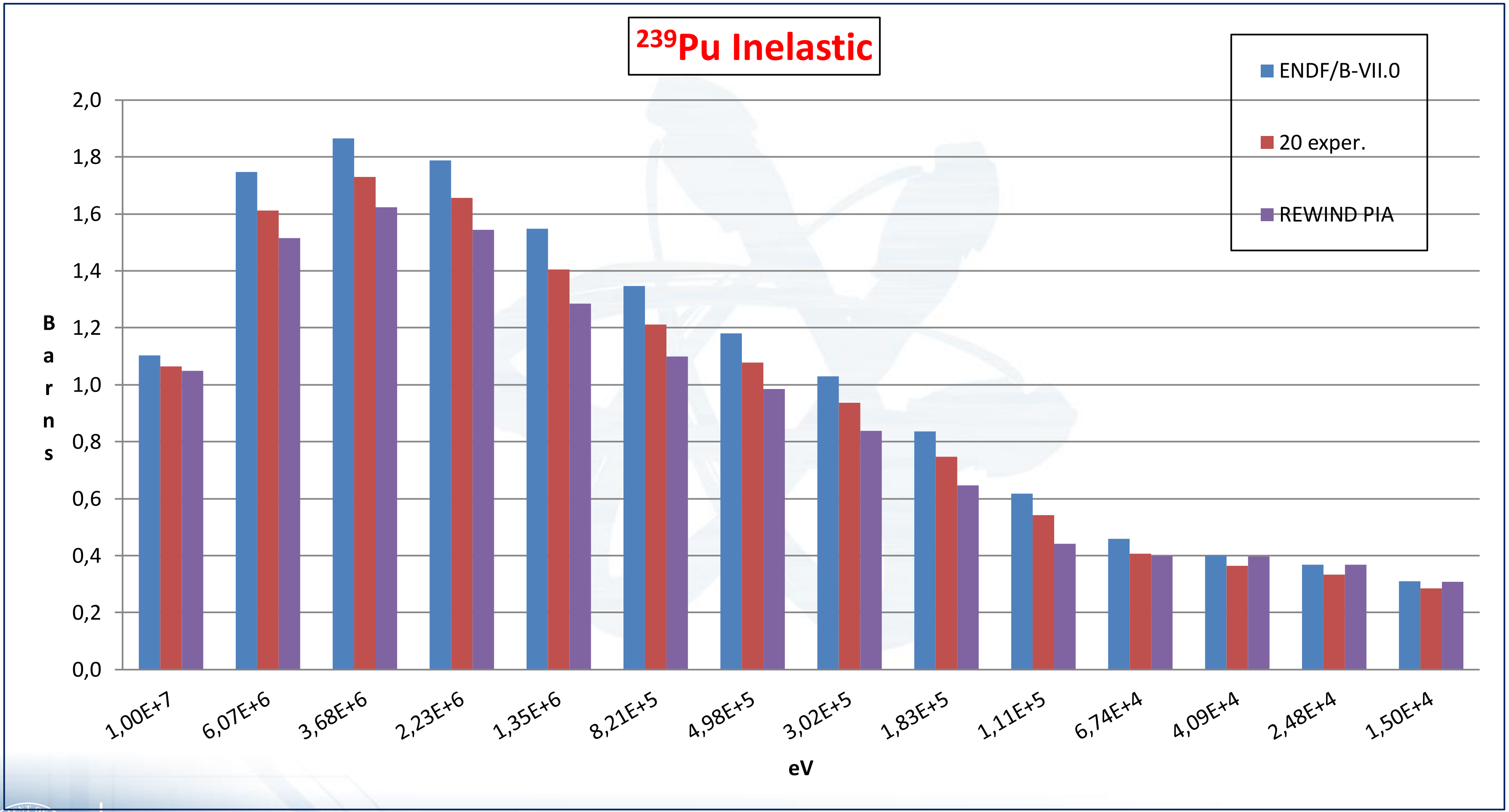
REWINDing PIA to SG33 experiments
σ



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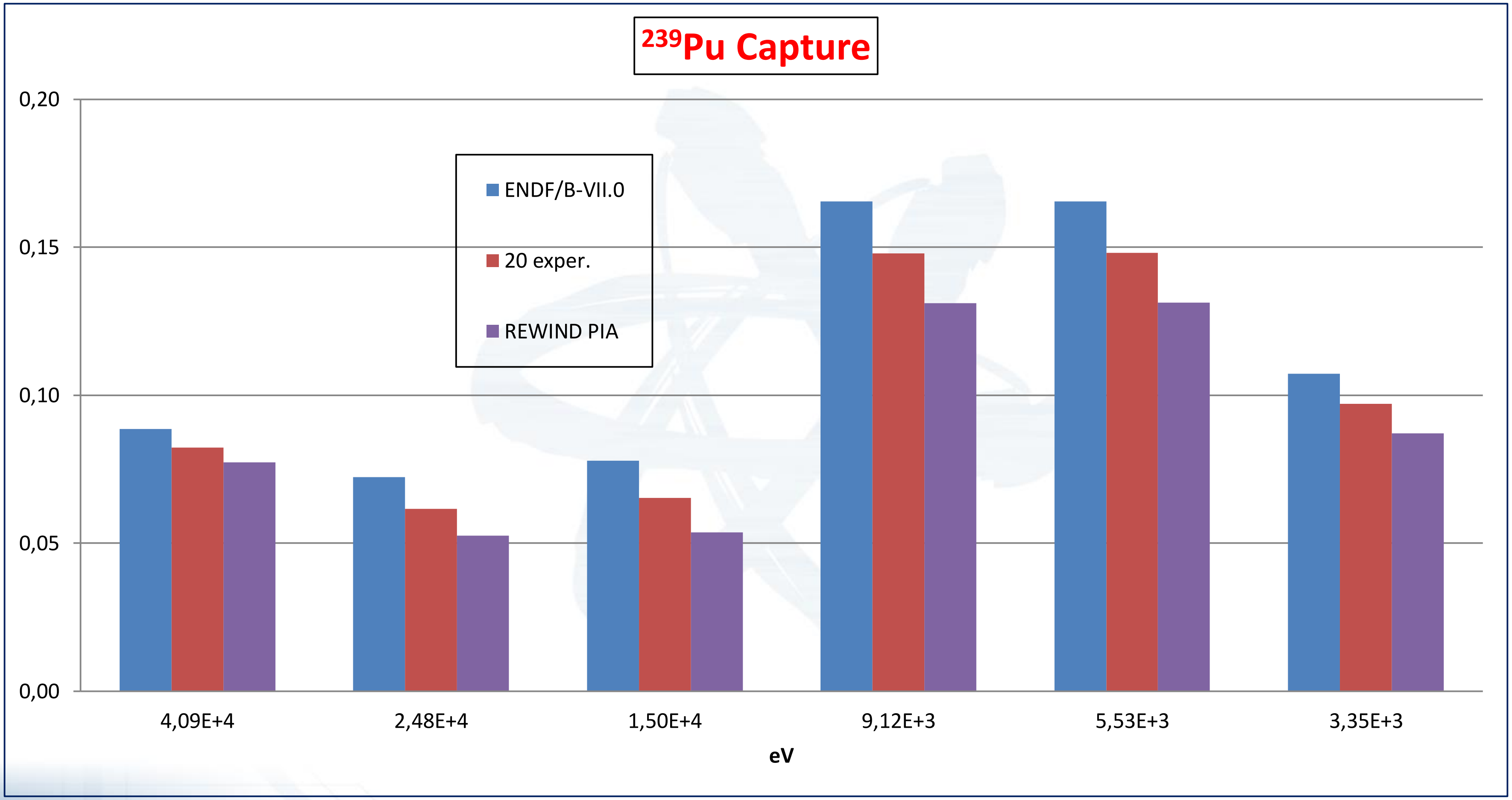
REWINDing PIA applied to SG33 experiments Standard Deviation



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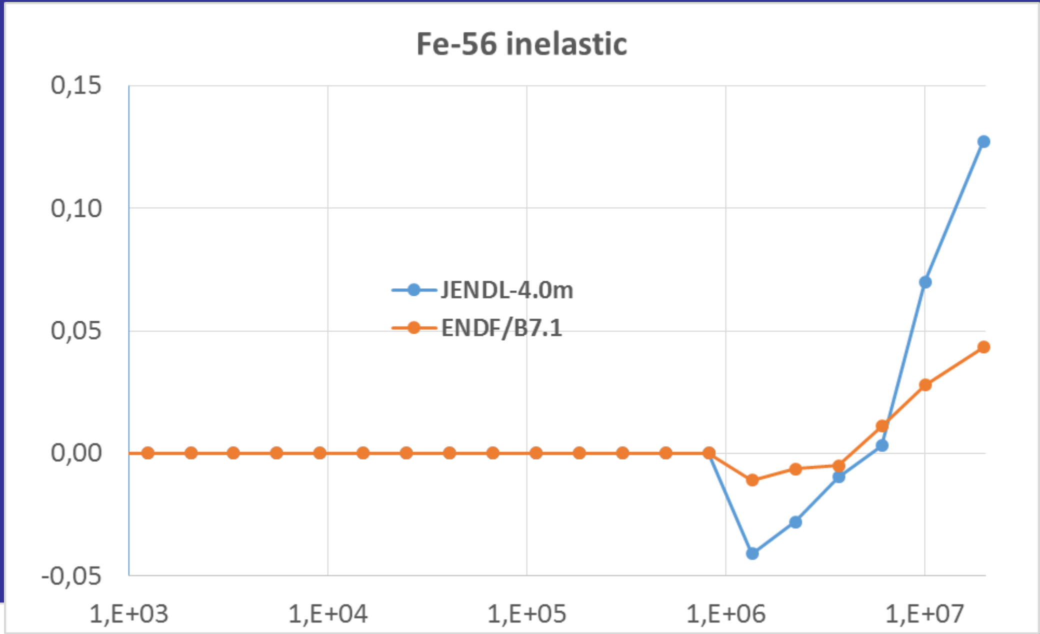
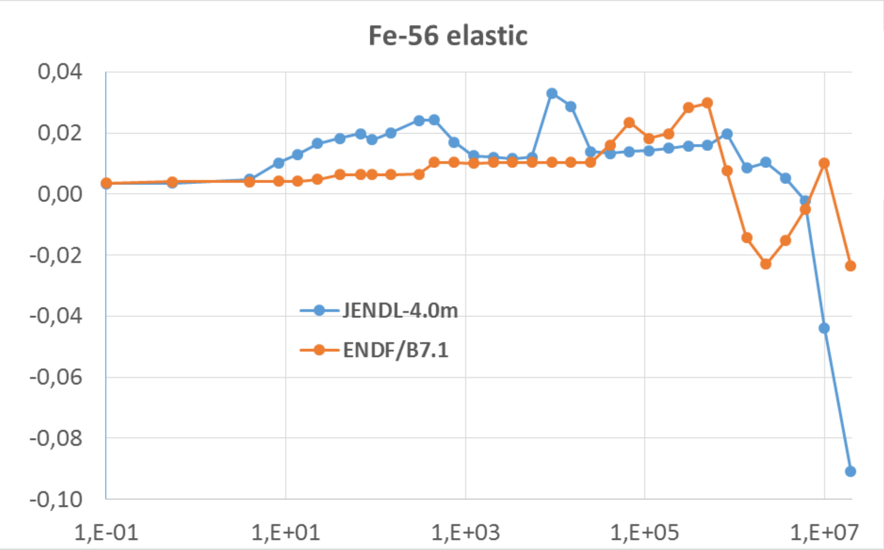
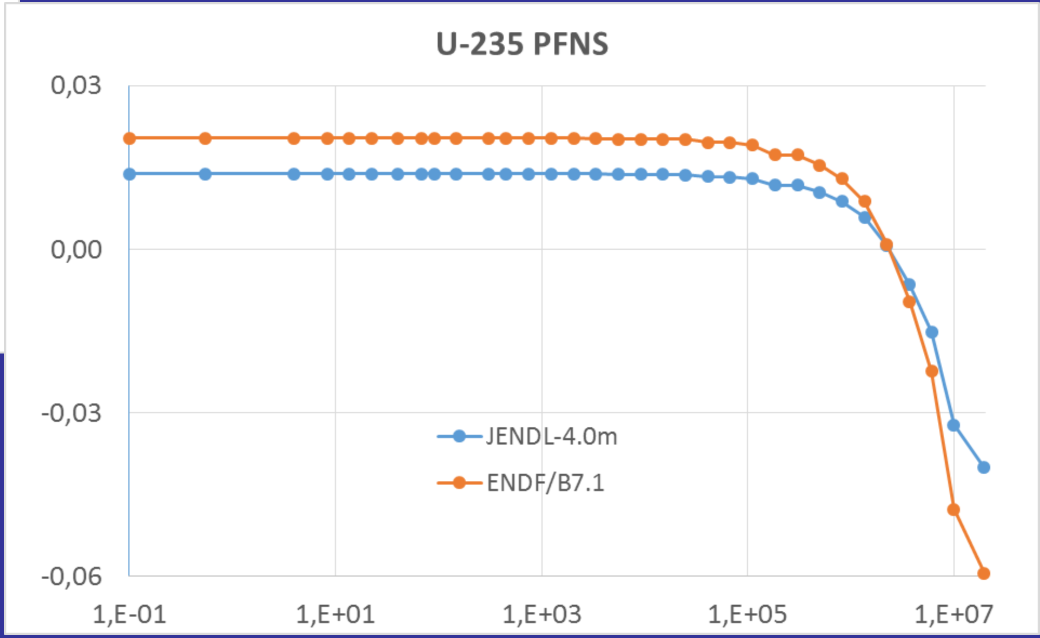
Examples of the results of adjustment exercise:
JENDL-4.0 vs. ENDF/BVII.1

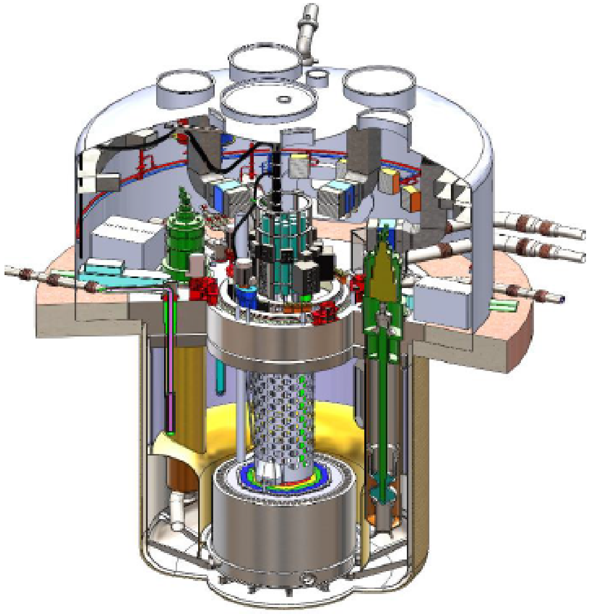






Background

- TerraPower was started by Bill Gates, Nathan Myhrvold, others after invention session in 2006. Privately funded.
- Goal: investigate advanced fission reactors for world-scale energy production
- Key requirements included high fuel utilization, low barriers to exportation, enhanced safety, and improved cost
- Traveling Wave Reactor was chosen
  - "Breed-and-burn" concept enables fast reactor without reprocessing
  - Has been discussed in literature since at least 1958
- Leveraging worldwide SFR experience allows quickest commercialization



Key Challenges in TWR Development

- Very high burnup fuel (~30 %FIMA peak)
- Very high neutron dose on cladding, duct (>500 DPA peak)
- Large, low-leakage core with high void worth

TerraPower

TWR-P Uncertainty Results

Nominal values of key TWR-P integral parameters with uncertainties due to nuclear data

Integral Parameter	Nominal BOL	Nominal EOL	Uncertainty BOL	Uncertainty EOL
k_{eff}	0.997488	0.997980	2.24E-02	1.59E-02
Coolant temperature coefficient (₵/K)	3.62E-03	4.90E-02	4.99E-03	5.64E-03
Doppler coefficient (₵/K)	-8.27E-02	-9.43E-02	4.77E-03	4.82E-03
Void worth ($)	2.42E-01	3.33E+00	3.55E-01	3.82E-01
Control Rod worth ($)	-1.02E+00	-1.45E+00	2.99E-02	3.78E-02

Relative uncertainties due to nuclear data in key TWR-P integral parameters

Integral Parameter	TWR-P BOL	TWR-P EOL
k_{eff}	2.25E-02	1.59E-02
Coolant temperature coefficient	1.38E+00*	1.15E-01
Doppler coefficient	5.77E-02	5.11E-02
Void worth	1.47E+00	1.15E-01
Control Rod worth	2.92E-02	2.61E-02

* Note high relative uncertainty due to very small absolute

Conclusions

Key nuclides/reaction uncertainties:

- ^{235}U capture
- ^{238}U inelastic scatter cross
- ^{23}Na scattering cross sections (both elastic and inelastic) contribute significantly to void worth, Doppler, and CTC uncertainties.
- ^{235}U PFNS (χ) and ^{56}Fe elastic scatter

For TWR-C, the priority list is very similar, but ^{239}Pu χ replaces ^{235}U in the list.

Next Steps and Needs

Near-term

- Redo with ENDF/B-VII.1 library for MC**2-3, or alternative lattice code
- Implement sensitivity coefficients for more integral parameters (power density, etc.)
- Implement propagation of uncertainty with depletion, and through other physics modules
- Communicate key energies/reactions to experimenters and evaluators

Longer-term

- Perform data assimilation to reduce uncertainties with TWR-P target
  - Includes study of representativity of available experiments to TWR
- Coordinate experiments if necessary to fill in gaps

ACKNOWLEDGMENTS

The author acknowledges coaching from M. Salvatores and G. Palmiotti. Additionally, the continuing work of NEA/WPEC subgroups 26, 33, 39 and 40 has proved invaluable to this effort. Thanks also to Jeremy Conlin for his help extracting the ^{235}U MF35/MT18 file.

Future Actions

- **Perform extended adjustment using more elemental type of integral experiments and new adjustment strategies in order to provide more useful feedback to CIELO isotopes.**
- **Improved criteria for reliability (from methodology studies).**
- **Provide impact on existing selected experiments by the new evaluated CIELO isotopes (ENDF/B-VIII.0 βx) and corresponding JEFF3.3 isotopes: by energy range, reaction, and isotope.**
- **Continue to develop continuous energy data assimilation techniques.**
- **In order to provide more reliable and useful feedback, we need more complete covariance information, possibly cross correlations, angular distributions, secondary energy distributions, delayed data, etc.**

Summary

- **The subgroup is very active and many, very useful, contributions have been produced by the participants.**
- **One intermediate deliverable has been finalized and two others should be available soon.**
- **The main focus is concentrated on dealing with compensations and more efficient data assimilation methodologies:**
  - **Adding more experiment of elemental type and/or of separation effect type.**
  - **Developing new adjustment strategies and methodologies.**
  - **New emerging needs, customer driven, are considered.**
- **Expecting feedback from CIELO in terms of more complete and reliable covariance data in the next future.**