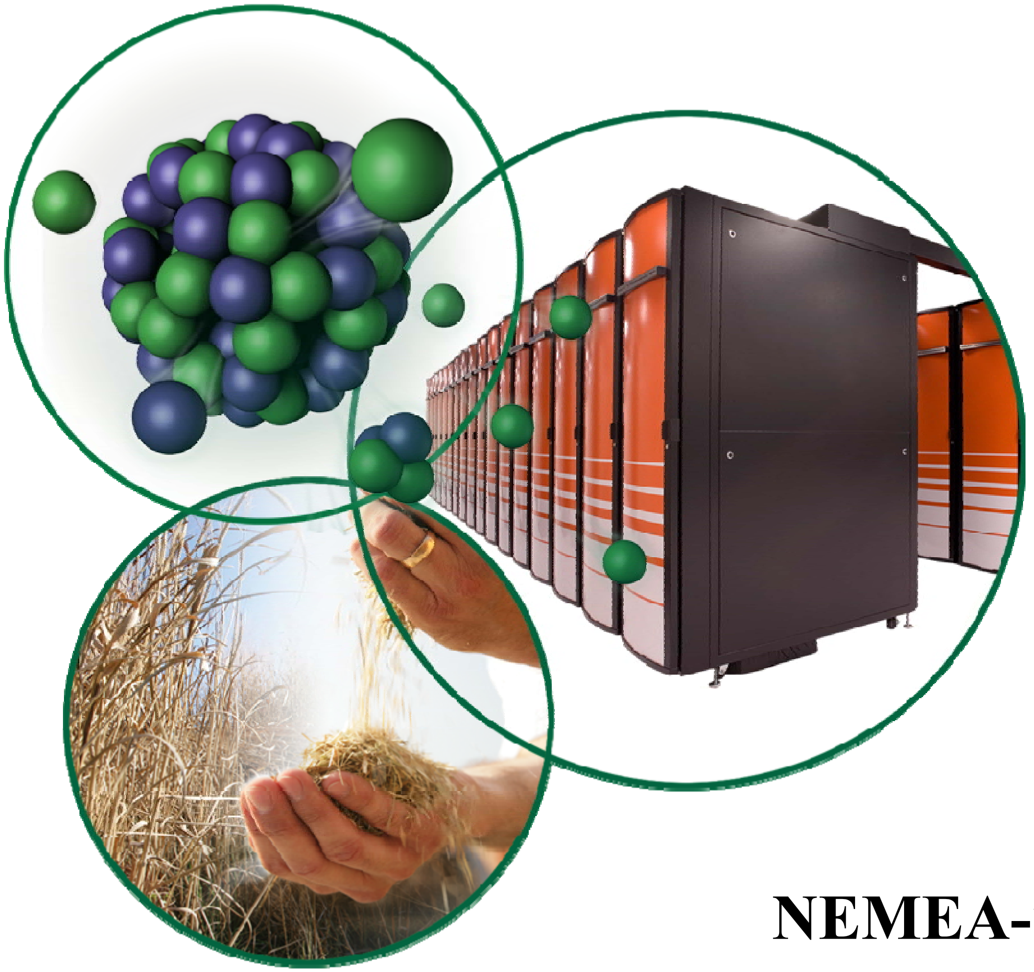
Resonance Evaluations of ^{235}U for the CIELO Project



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2) Los Alamos National Laboratory

3) CEA/Cadarache

NEMEA-7/CIELO Workshop
November 5-8, 2013

OUTLINE

Presentation will be performed in four parts:

1)^{235}U Evaluation and its Evolution

2)New Evaluation of the Resolved Resonance Range and Benchmark results

3)New Evaluation of the Unresolved Resolved Range and Benchmark results

4)Preliminary investigation of the two-step (n,γf) reaction

First Part
^{235}U Evaluation and its Evolution

^{235}U Evaluation an its Evolution

ENDF/B-V ^{235}U Resolved Resonance (RR)

- **RR range: 10^{-5} eV – 81eV**
  - E < 1 eV: smooth cross section (FILE 3)
  - 1 eV < E < 81 eV: Single-Level Breit-Wigner + smooth cross section (FILE 3)
- **RR evaluation based on analysis done by Smith & Young for ENDF/B-III (1970)**
- **Level-spin information not included!!**

Motivation for a new ^{235}U Evaluation

- **Multilevel R-matrix Reich-Moore formalism being developed in the SAMMY code;**
- **Use of the Bayesian approach to allow the analysis of several experimental data sequentially;**
- **Direct introduction of experimental condition in the evaluation: sample thickness, broadening parameters, normalization, etc;**
- **Availability of spin-separated data by Keyworth et al.**
- **New high resolution transmission data and fission cross section done at ORELA;**

ENDF/B-VI ^{235}U RR Evaluation

- **Due to computer limitations decision was made to split the resonance evaluation on seven disjoint energy ranges from 10^{-5} eV to 2250 eV;**
- **Use high-resolution transmission done by Harvey et al;**
- **Use high-resolution fission cross section done by Weston, Gwin, Spencer, etc;**
- **Use spin-separated data for determine s-wave total angular momentum 3^- and 4^-;**
- **No new capture measurements were done!!**
- **Use delta-3 statistics for helping identifying missing levels;**

Experimental Data Base

Author	Energy (eV)	Data
De Saussure (RPI/1967)	0.01 - 2250.0	Fission and Capture at 25.2 meters
Perez (ORNL/1972)	0.01 - 200.0	Fission and Capture at 39.7 meters
Weston (ORNL/1984)	14.0 - 2250.0	Fission at 18.9 meters
Gwin (ORNL/1984)	0.01 - 20.0	Fission at 25.6 meters
Spencer (ORNL/1984)	0.01 - 1.0	Transmission at 18 meters and sample thickness of 0.001468 atom/barn
Harvey (ORNL/1986)	0.4 - 68.0	Transmission at 18 meters and sample thickness of 0.03269 atom/barn

Experimental Data Base

Author	Energy (eV)	Data
Harvey (ORNL/1986)	4.0 - 2250.0	Transmission at 80 meters and sample thickness of 0.00233 atom/barn cooled to 77 K
Harvey (ORNL/1986)	4.0 - 2250.0	Transmission at 80 meters and sample thickness of 0.03269 atom/barn cooled to 77 K
Wartena (Geel/1987)	0.0018 - 1.0	Eta at 8 meters
Wagemans (Geel/1988)	0.001 – 0.4	Fission at 18 meters
Schrack (RPI/1988)	0.02 - 20.0	Fission at 8.4 meters
Weigman (ILL/1990)	0.0015 – 0.15	Eta (Chopper)

Experimental Data Base

Author	Energy (eV)	Data
Weston (ORNL/1992)	100.0 - 2000.0	Fission at 86.5 meters
Moxon (ORNL/1992)	0.01 - 50.0	Fission Yield
Gwin (ORNL/1996)	0.01 - 4.0	Absorption and fission at 21.68 meters

Issues with the ^{235}U RR Evaluation

- Evaluation released as ENDF/B-VI.0
- No benchmark test were done prior to the evaluation release;
- Despite the good differential data fitting the evaluation did not do well in benchmark calculations. Results deteriorated compared to ENDF/B-V results, indeed;

Attempt to fix the ^{235}U RR Evaluation

- **Lubitz performed an excellent job indicating key integral parameters to improve the evaluation;**
- **K1 value was key to the evaluation for thermal benchmark calculations;**
- **Work was done based on the seven disjoint sets of resonance parameters;**
- **No fit of the differential data was done;**
- **Evaluation released to ENDF**

Present ^{235}U RR Evaluation

- Computer resources more efficient to allow one set of resonances in the energy range 10^{-5} eV to 2250 eV;
- Inclusion of integral data in the SAMMY fitting (K1, Westcott factors, etc.);
- New measurements of η at low energy to address Doppler coefficient of reactivity prediction;
- Evaluation should be tested nationally and internationally;
- Evaluation was released as ENDF/B-VI.3

WPEC subgroup 18:
"Epithermal Capture Cross Section for ^{235}U"

Quote from SG18:

"Release 6.3 did not do well on intermediate-spectrum cores, however, calculating 1-2% high on the HISS (HUG) and the two UH3 benchmarks which RQ Wright had added to the set being used to test 235U. It is possible that the "low-alpha syndrome" which affected Release 6.2 below 900 eV extends up higher in energy, but the results are also sensitive to possible errors in nubar."

- **Benchmarks in the intermediate energy region were not available the time ^{235}U ENDF/B-VII.3 was released;**
- **WPEC Subgroup 29 indicated issues !!**

WPEC subgroup 29:

"Uranium-235 Capture Cross-section in the keV to MeV Energy Region"

Mission:

- Investigate C/E discrepancies in uranium-core integral parameters observed with all major evaluated libraries (ENDF, JENDL, JEFF);
- Perform sensitivity analyses of integral parameters with respect to differential data;
- Review the ^{235}U capture cross-section to determine recommended values in the energy region from 100 eV to 1 MeV;
- Perform Benchmark calculations for the FCA-IX-1, -2 and -3 cores and the ZEUS-1, -2, -3, and -4;

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2nd part
New Evaluation of the Resolved Range and Benchmarking

^{235}U Issues and Resolutions:

Issues:

Overestimation of ^{235}U capture cross-section in the resonance region range (0.1 to 2.5 keV).

It is recommended:

i) New measurements of capture and fission cross-section in the keV region;

ii) Perform new resonance analysis in the 0.1 to 2.5 keV region;

iii) Investigate the reason for the overestimation of criticalities for some benchmarks.

^{235}U Issues and Resolutions:

Resolution:

✓ **New data measurements from RPI (capture and fission yields) (kind of alpha measurements);**

✓ **New capture data from LANL;**

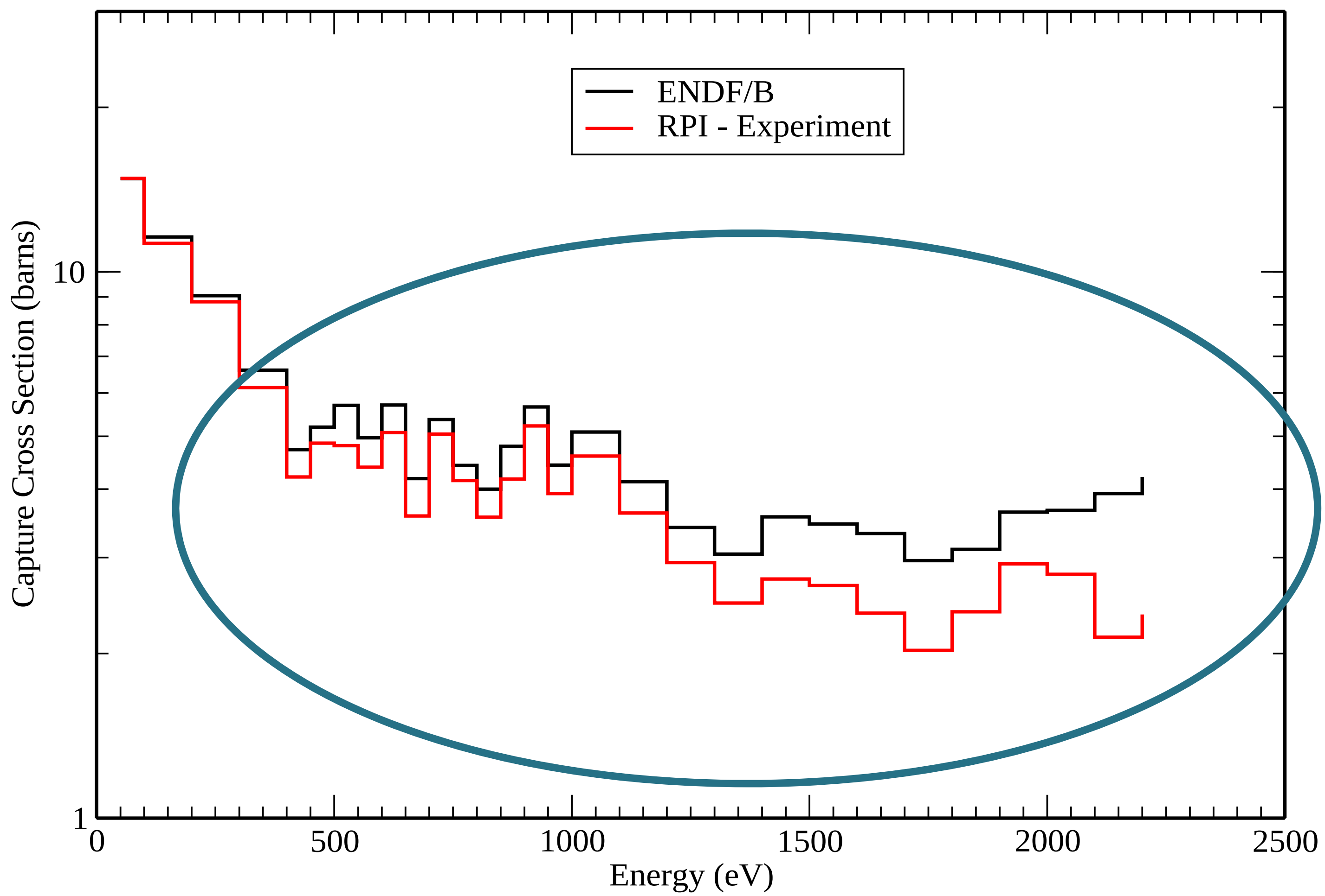
✓ **Use SAMMY code for fitting the new data;**

✓ **Test the new evaluation in benchmark calculations: ZEUS benchmarks (FCA not available);**

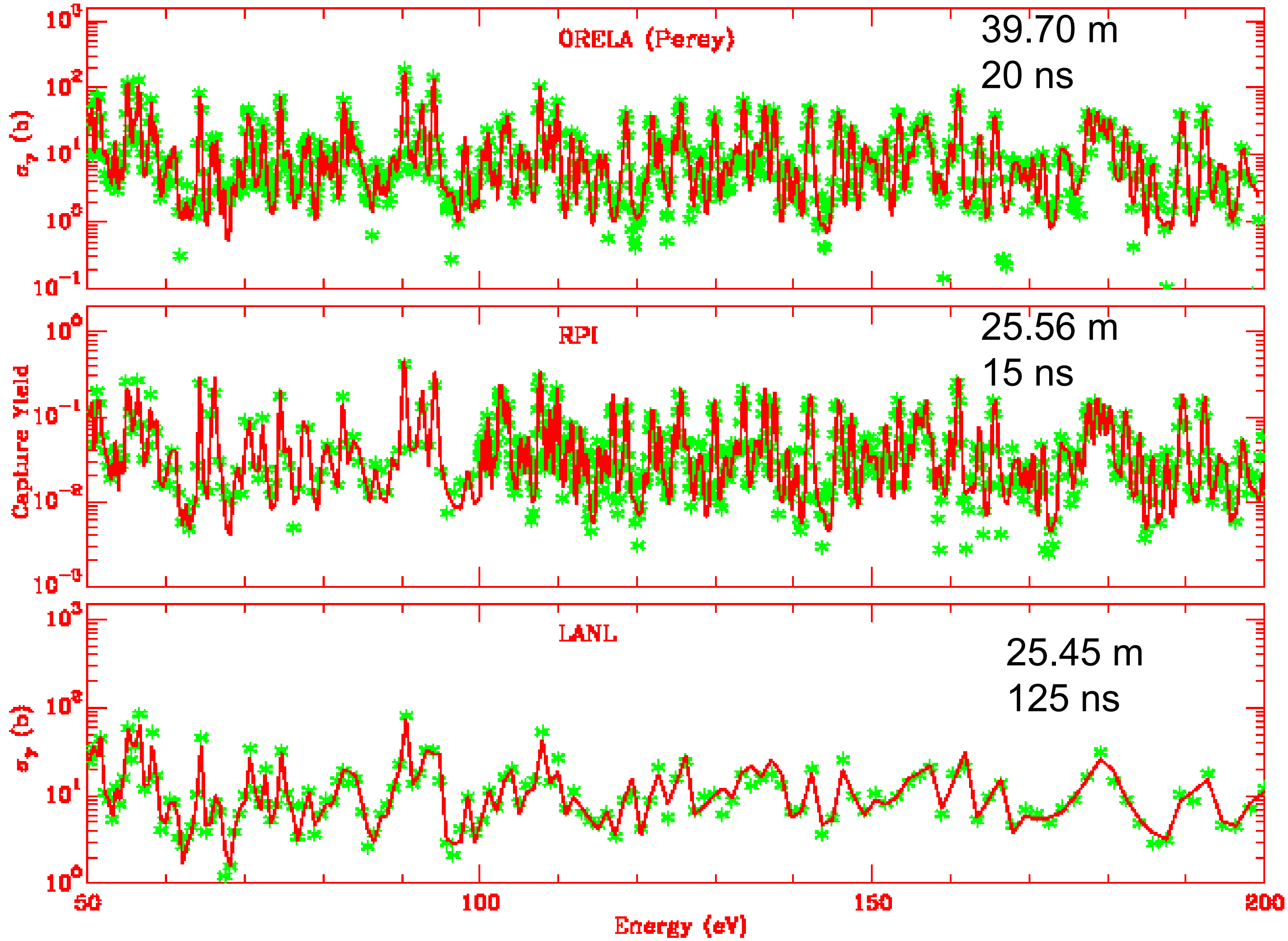
✓ **Use JENDL4 as the template;**

✓ **Benchmark Calculations done with MCNP with everything else from ENDF/B-VII.0;**

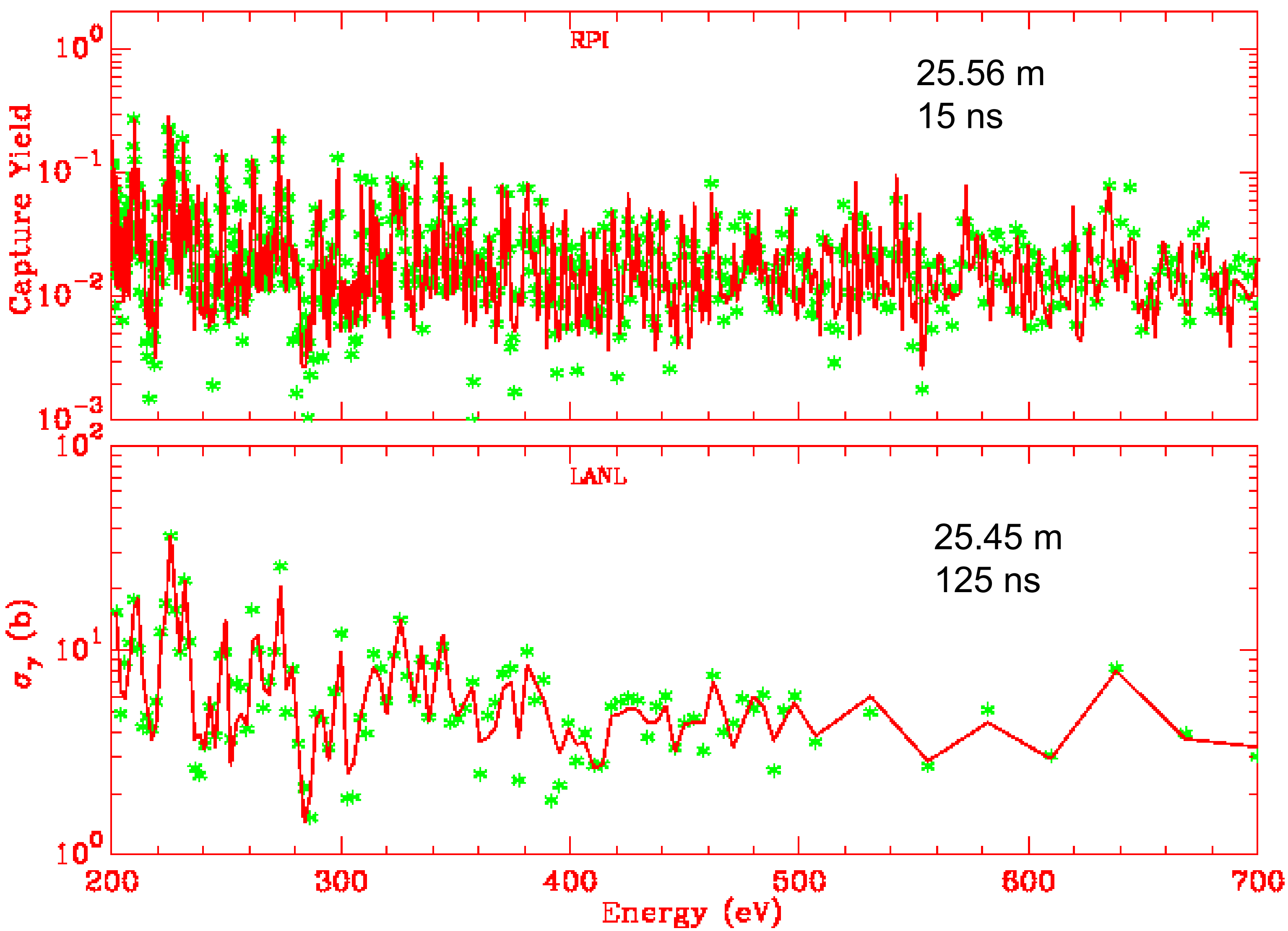
RPI capture data and ENDF evaluation (sg29 prediction confirmed)



ORNL, RPI and LANL Capture Data



RPI and LANL Capture Data



Selected Measurements ^{235}U

- **Four transmission measurements, eight fission cross section measurements and four capture cross section measurements were used in the evaluation;**
- **Evaluation performed up 2250 eV with 3197 resonances with 3168 in the energy range analyzed and 29 external resonances;**
- **Evaluation done using SAMMY with the Reich-Moore formalism;**
- **Fitted also integral data such as K1, Westcott factor, capture resonance integral;**

Selected Measurements

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Gwin (ORNL/1996)	0.01 - 4.0	Absorption and fission at 21.68 meters
Danon (RPI/2012)	100.0 – 5000	Fission and capture yield at 25.56 meters (burst 15 ns)
Jandel (LANL/2012)	100.0 - 5000	Capture at 25.45 meters (burst 125 ns)

Integral Quantities

- **Wescott Factor** $$g_x = \frac{2\sigma_x}{\pi^{1/2}\sigma_{0x}}$$
- **K_1 Parameter** $$k_1 = \upsilon\sigma_{0f}g_f - \sigma_{0a}g_a$$
- **Resonance Integral** $$I_x = \int_{0.5eV}^{20Mev} \frac{\sigma_x}{E} dx$$
- **Eta** $$\eta = \frac{\nu\sigma_f}{\sigma_a}$$

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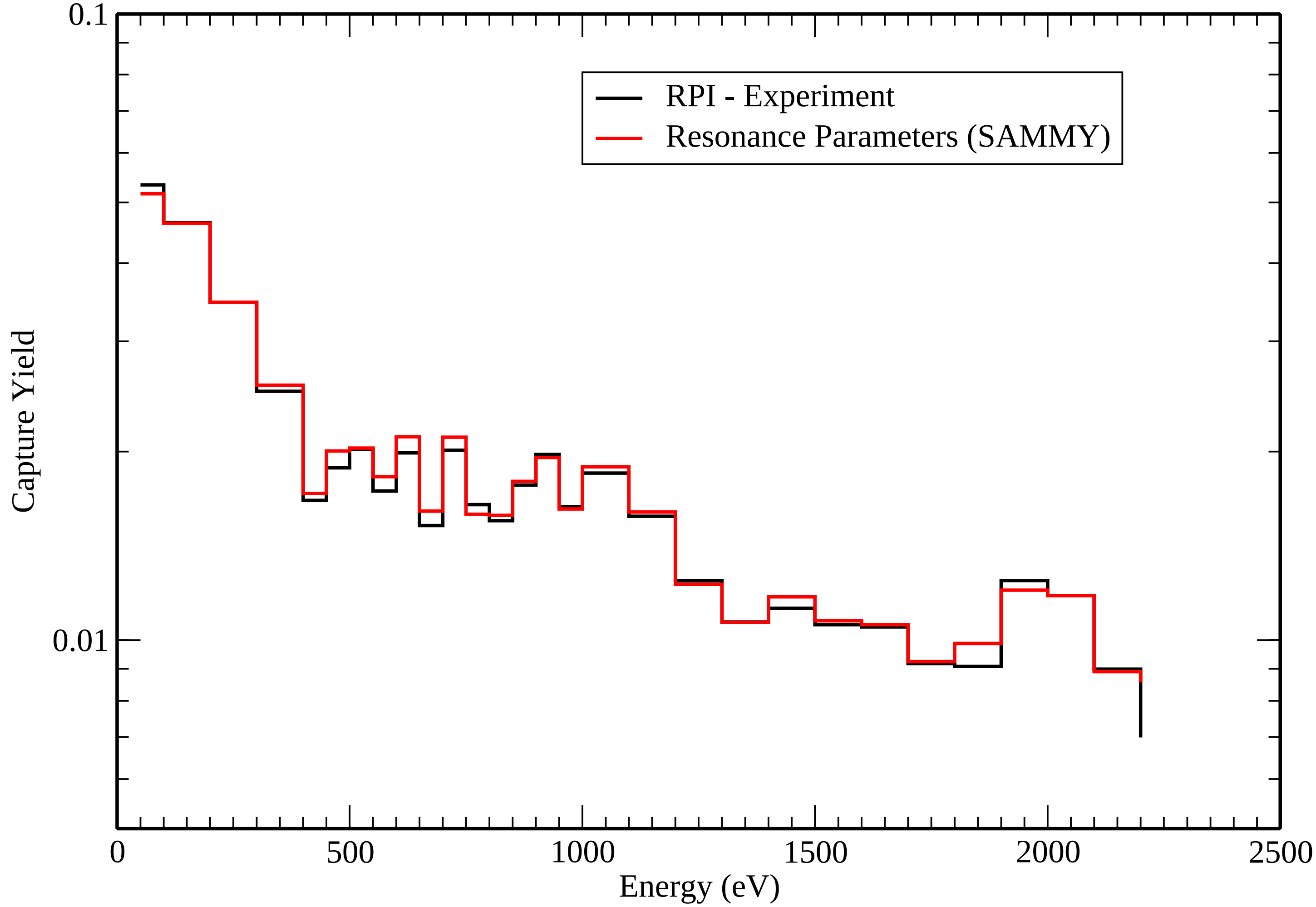
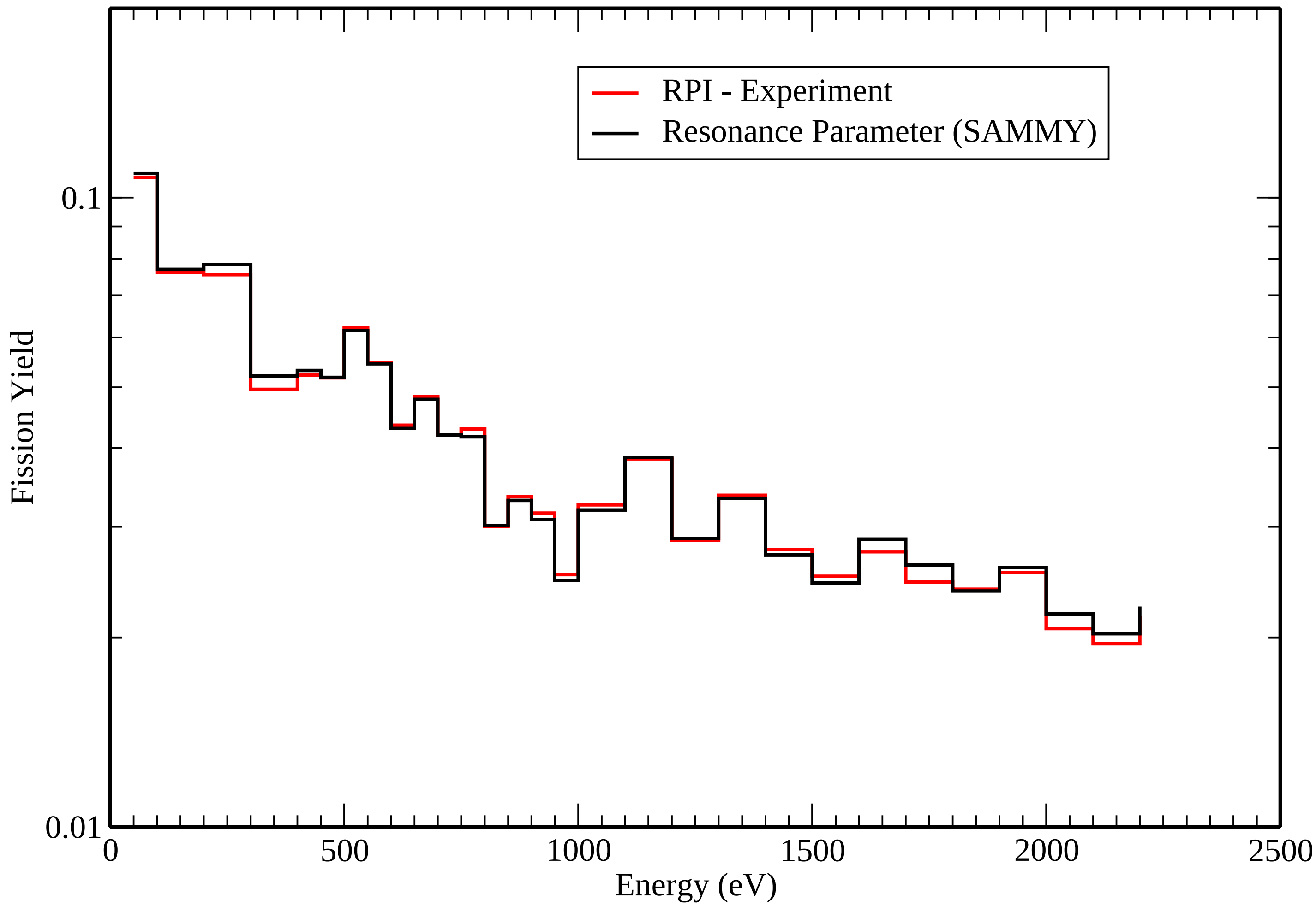
Fit of the RPI Capture Data



Fit of the RPI Fission data



ICSBEP Benchmark Calculations
The HEU-MET-INTER-006 cases (ZEUS)

Intermediate Energy Benchmark:

Designed to test the ^{235}U cross sections in the intermediate energy range.

ISCEB description:

- ✓ heu-met-inter-006-1 (ZEUS1)
- ✓ heu-met-inter-006-2 (ZEUS2)
- ✓ heu-met-inter-006-3 (ZEUS3)
- ✓ heu-met-inter-006-4 (ZEUS4)

The HEU-MET-INTER-006 cases (ZEUS)

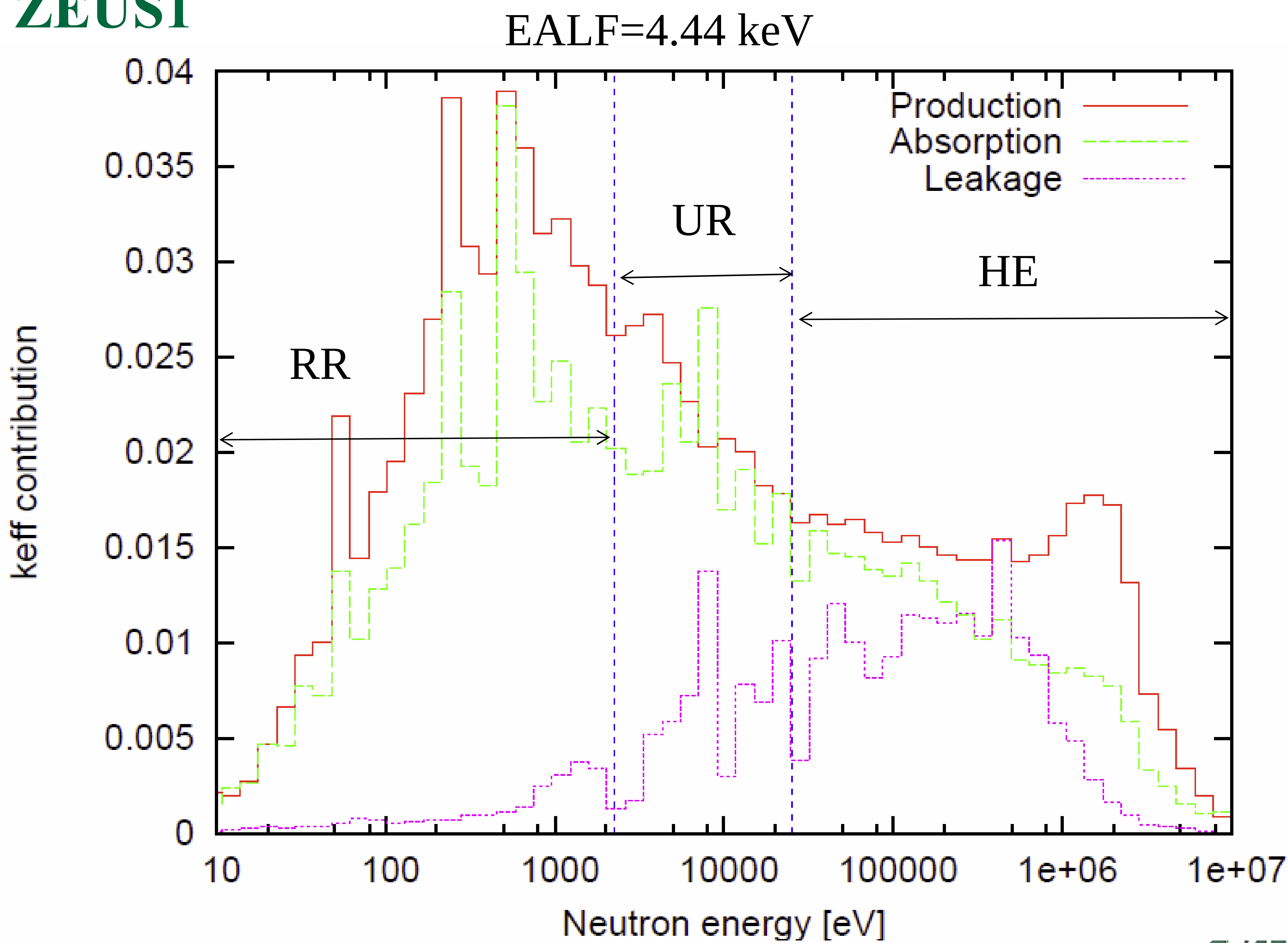
Case Number	k_{eff}	EALF (keV)	Intermediate-Energy Fission Fraction
1 (ZEUS1)	0.9977 ± 0.0008	4.44	0.730
2 (ZEUS2)	1.0001 ± 0.0008	9.45	0.698
3 (ZEUS3)	1.0015 ± 0.0008	22.80	0.636
4 (ZEUS4)	1.0016 ± 0.0008	80.80	0.503

EALF: Energy Average Lethargy Causing Fission

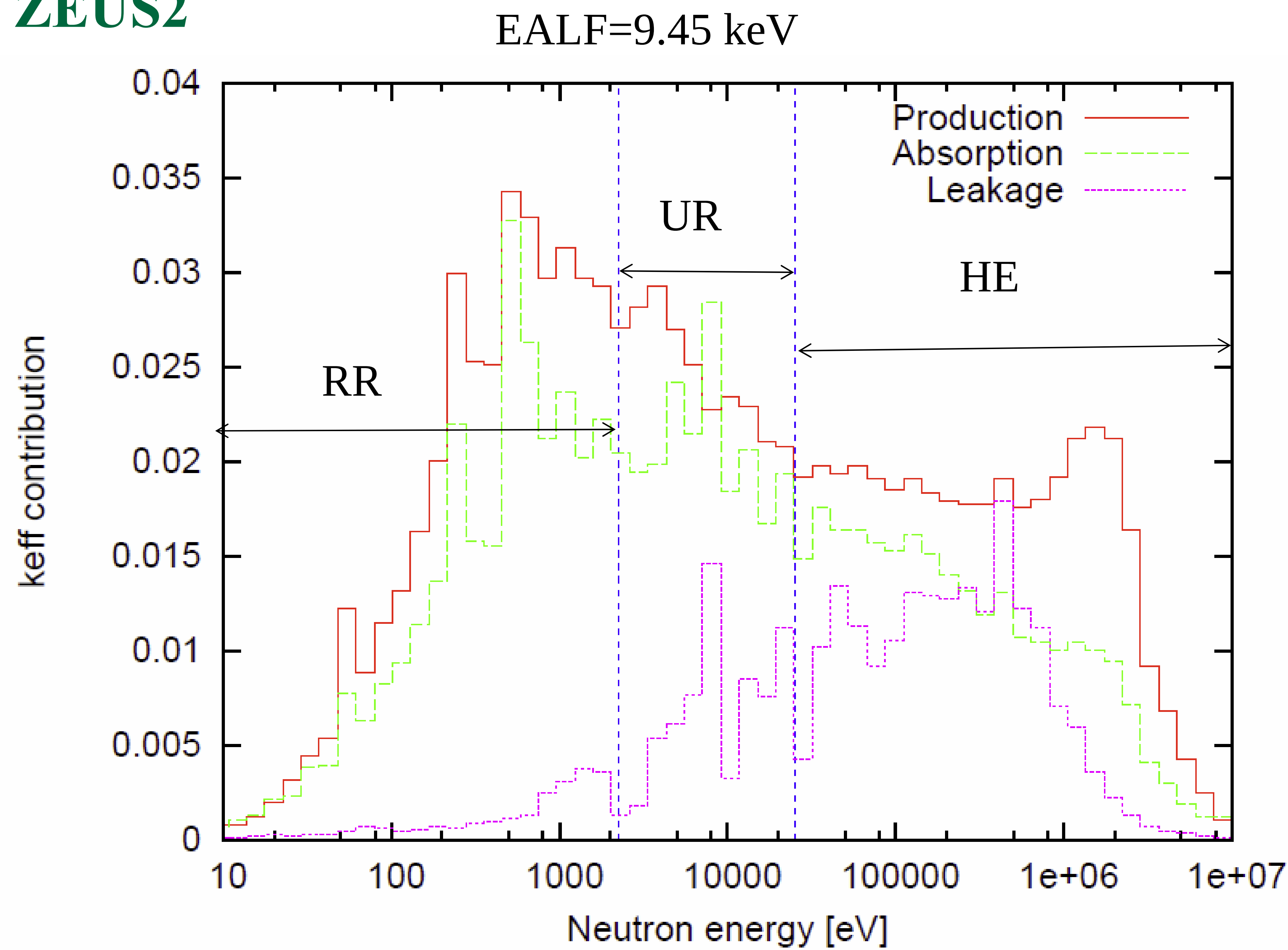
Effective System Multiplication Factor

$$k_{eff} = \frac{\text{Production}}{Absorption + Leakage}$$

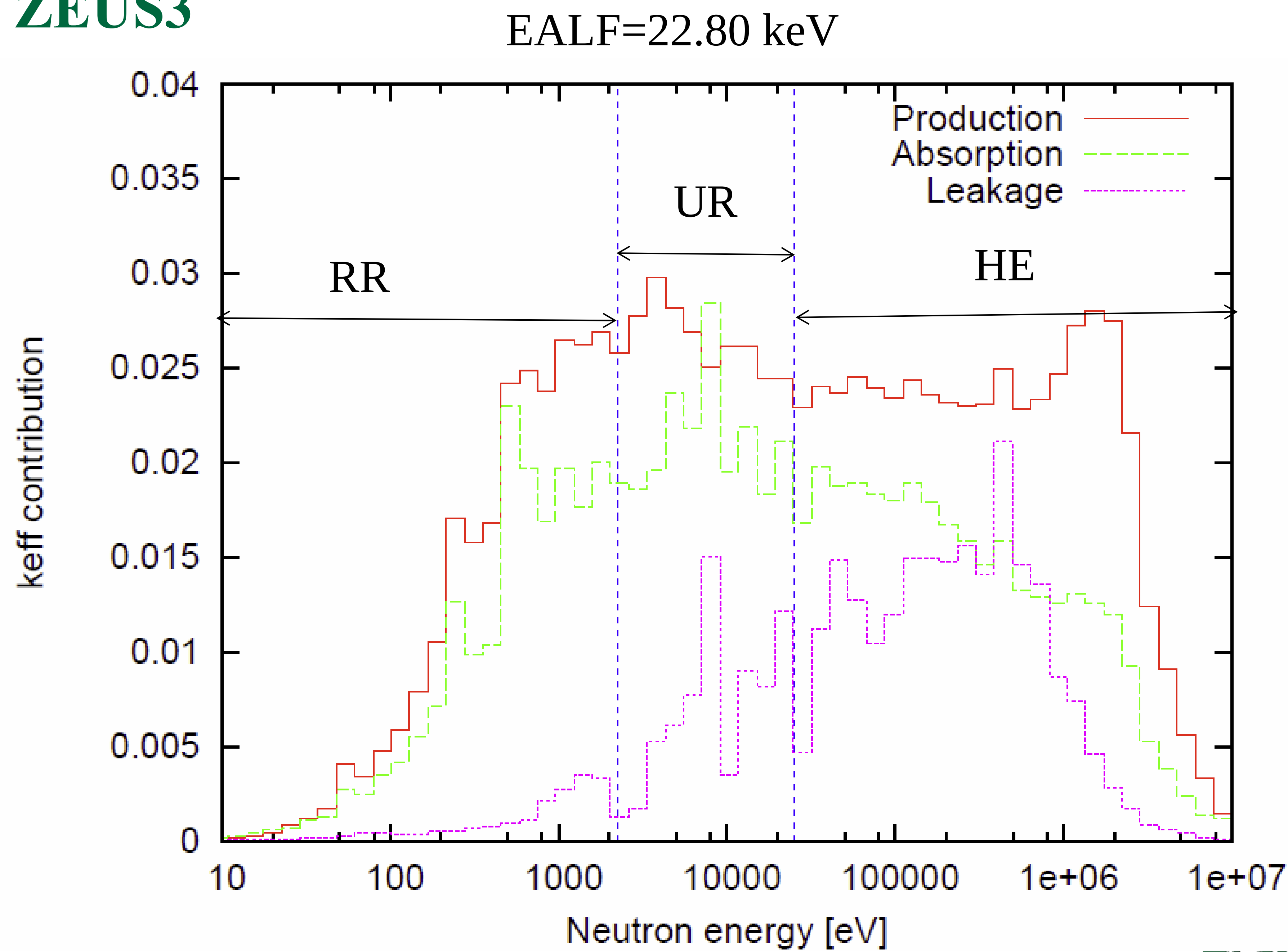
ZEUS1


EALF=4.44 keV
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
keff contribution
10
100
1000
10000
100000
1e+06
1e+07
Neutron energy [eV]
Production
Absorption
Leakage
RR
UR
HE

ZEUS2

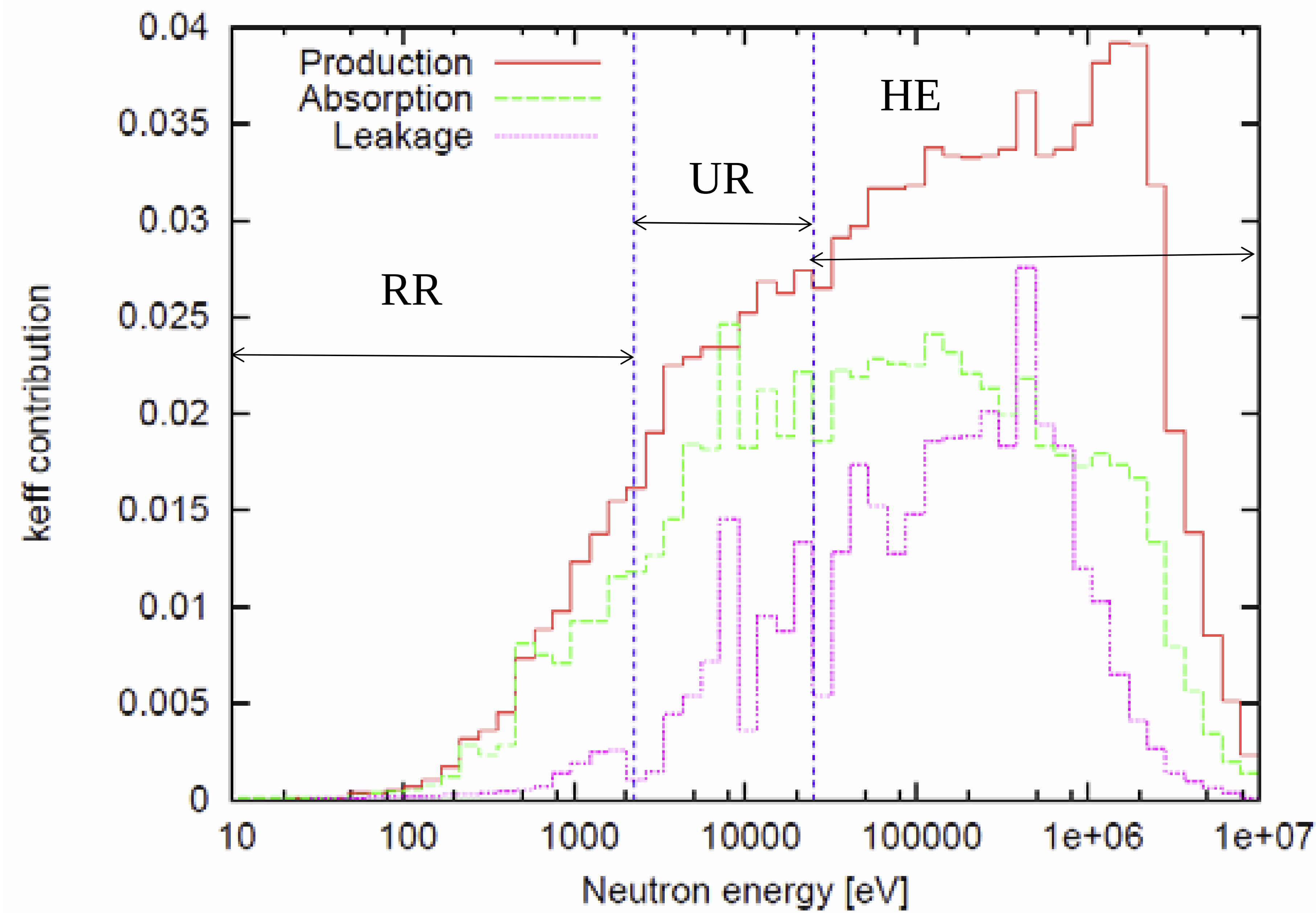

EALF=9.45 keV
keff contribution
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
10
100
1000
10000
100000
1e+06
1e+07
Neutron energy [eV]
Production
Absorption
Leakage
RR
UR
HE

ZEUS3


EALF=22.80 keV
keff contribution
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
10
100
1000
10000
100000
1e+06
1e+07
Neutron energy [eV]
Production
Absorption
Leakage
RR
UR
HE

ZEUS4

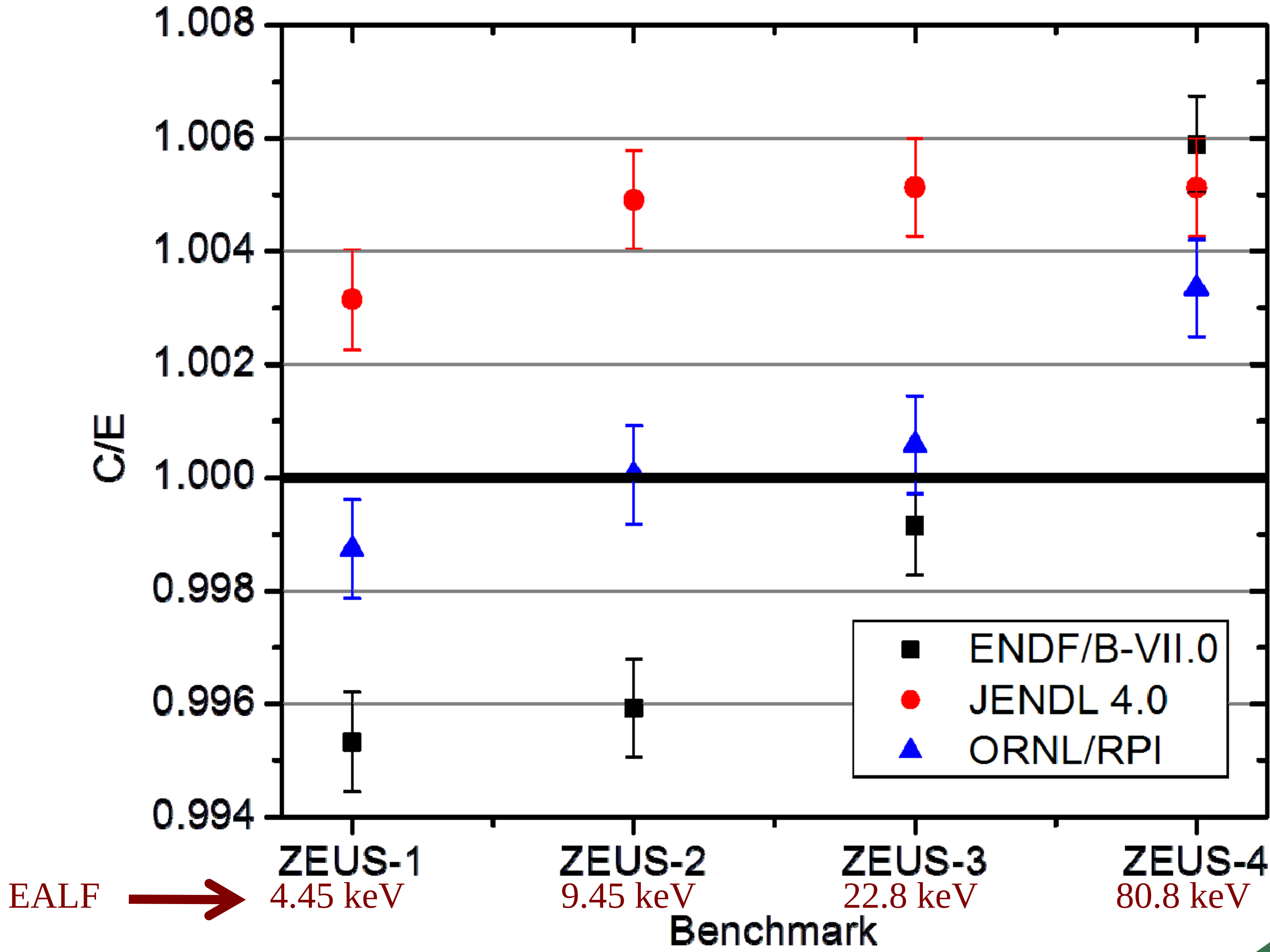
EALF=80.80 keV



The HEU-MET-INTER-006 cases (ZEUS)

Case Number	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII.0	JENDL4	ORNL
1 (ZEUS1)	0.9977 ± 0.0008	0.99304 ± 0.00035	1.00084 ± 0.00036	0.99644 ± 0.00035
2 (ZEUS2)	1.0001 ± 0.0008	0.99603 ± 0.00035	1.00501 ± 0.00036	1.00015 ± 0.00035
3 (ZEUS3)	1.0015 ± 0.0008	1.00065 ± 0.00035	1.00664 ± 0.00034	1.00208 ± 0.00033
4 (ZEUS4)	1.0016 ± 0.0008	1.00750 ± 0.00031	1.00673 ± 0.00034	1.00496 ± 0.00031

The HEU-MET-INTER-006 cases (ZEUS)



3rd part
New Evaluation of the Unresolved Resolved Range and Benchmarking

Integral Data Assimilation of the PROFIL and PROFIL-2 results

The α(U-235) ratio has been calculated for U-235 as a function of neutron energy by using the PROFIL and PROFIL-2 sample irradiation experiments carried out in the PHENIX reactor of the CEA/DEN Marcoule.

These experiments use rods with a large number of samples (~ 130 samples) containing almost pure separated actinides and fission products isotopes. They were designed to collect integral information for improving the neutron-induced cross sections of interest for fast reactor applications.

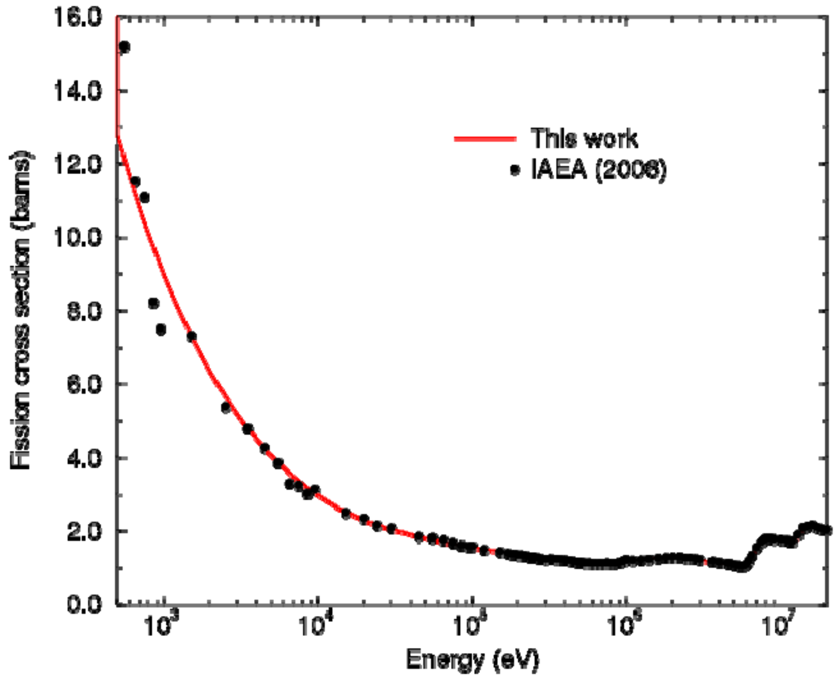
The PROFIL results were analysed using the ERANOS-2.2 code with the JEFF-3.1.1 nuclear data library. Such analyses show that the α(U-235) ratio can be derived from the (U-235/U-238) and (U-236/U-235) individual isotopic ratios, which characterize the U-235 fission and capture cross sections respectively.

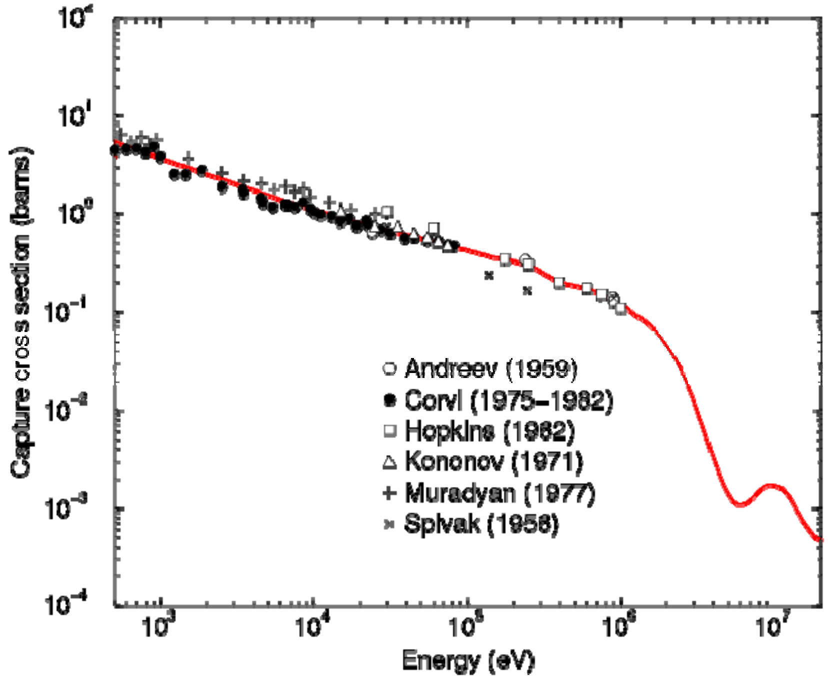
⇒The Integral Data Assimilation (IDA) procedure implemented in the CONRAD code allows the extraction of reliable α(U-235) ratio within the neutron energy range [500 eV - 150 keV]

⇒The ECIS and TALYS codes were used to calculate the neutron cross sections

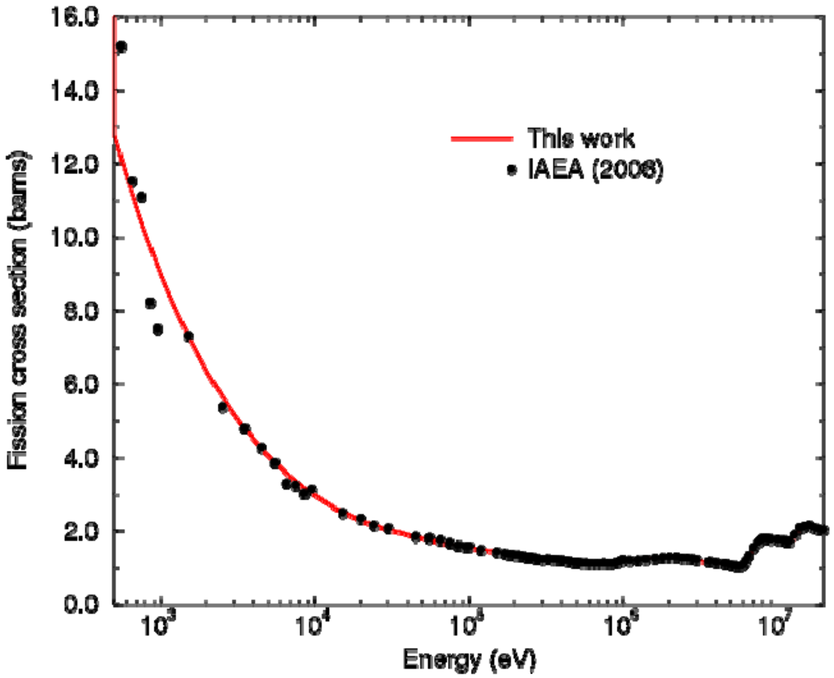
⇒JENDL-4 + ORNL evaluation used as a template

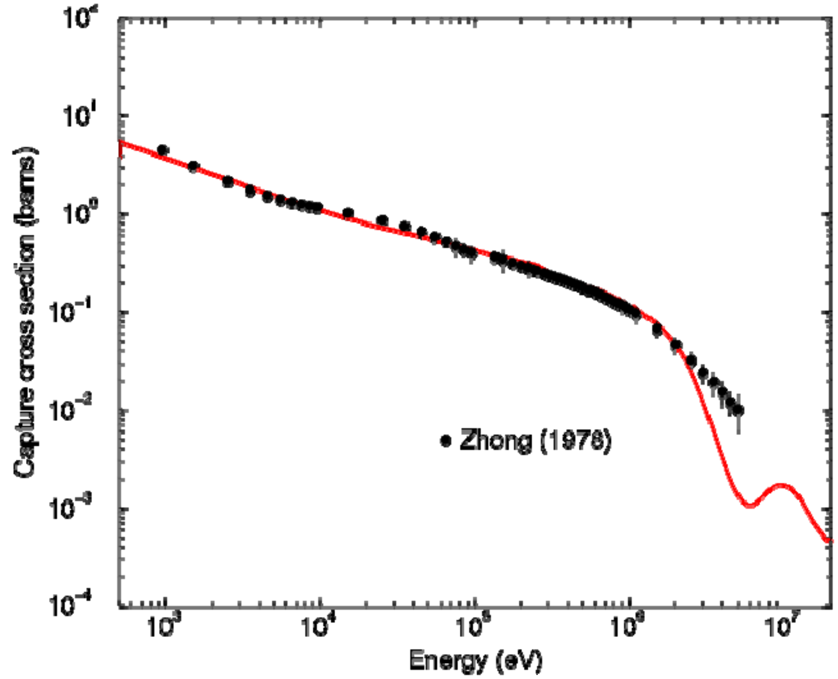
The capture cross section is deduced from α(U-235) by using the fission cross section recomended by the standard group of AIEA



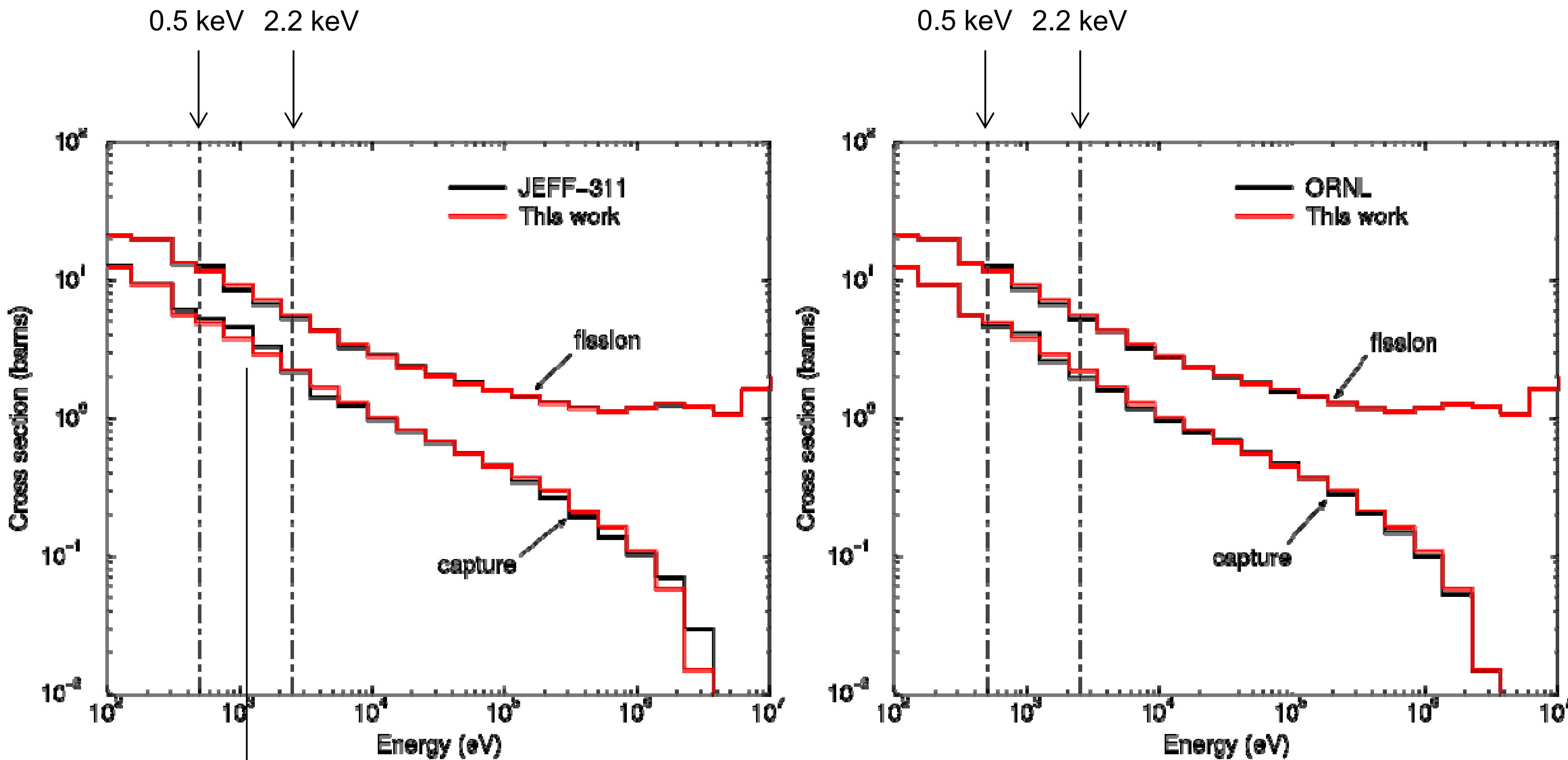


Below 100 keV, the capture cross section seems to be consistent with the older « evaluation » work of Zhong (1978)





Comparison of the broad group average cross sections



Statistical calculation seems to confirm the overestimation of the capture cross section in the keV energy range

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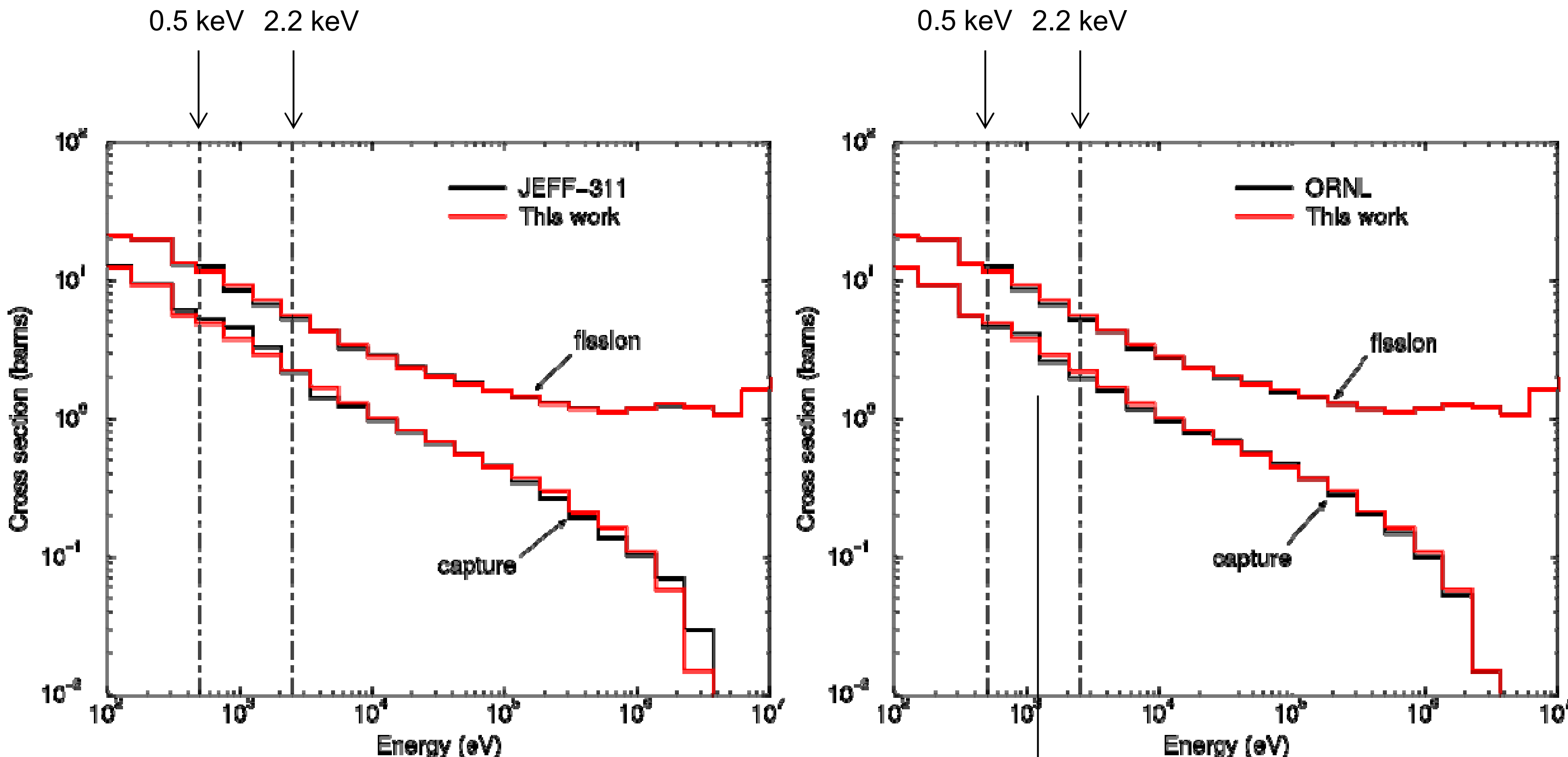
Comparison of the broad group average cross sections

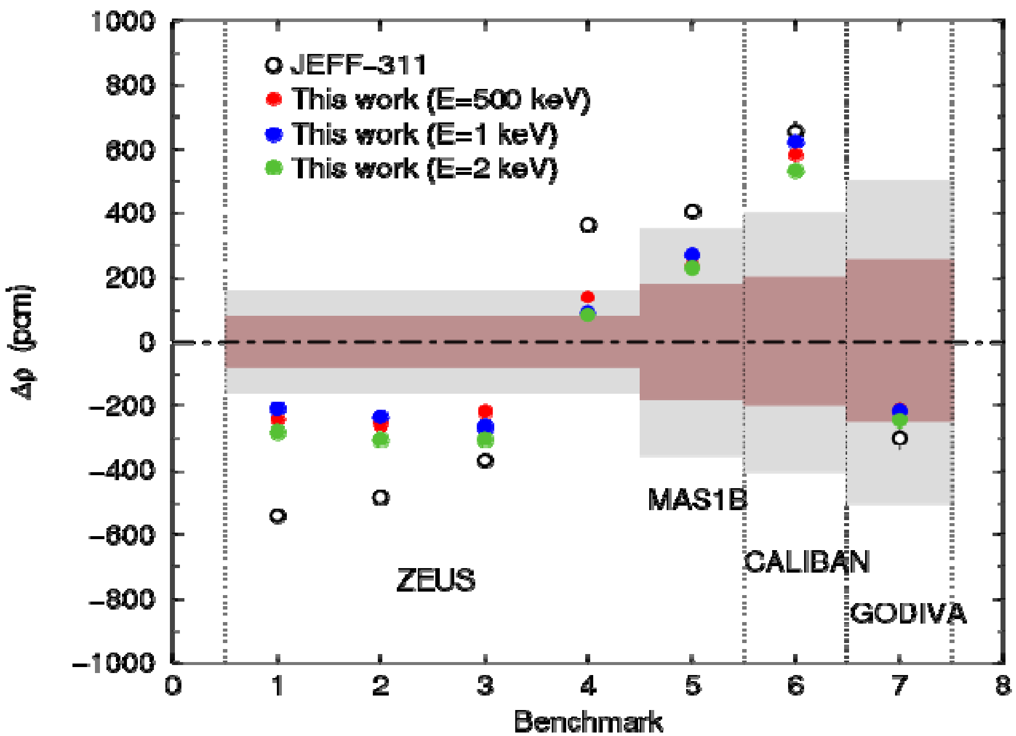


Good agreement with the new RRR evaluation from ORNL

Preliminary benchmark results (TRIPOLI calculations)

Three evaluated nuclear data files were tested with different upper energy limit for the RRR (500 eV, 1 keV and 2 keV) ⇒ no significant impact (« statistical » behavior of U235)

NB: the GODIVA uncertainty was updated according to work of P.M. Bess (ND2013)



⇒ For MAS1B, additional improvement is expected with new U238 from Capote et al.

4^{th} part
Preliminary investigation of the two-step (n,γf) reaction

Short list of references

1959 : unpublished estimation of the $\Gamma_{\gamma f}$ width for the (n,γf) reaction by E. Lynn

1965 : On the slow neutron, gamma-fission reaction, E. Lynn, Phys. Lett. 18

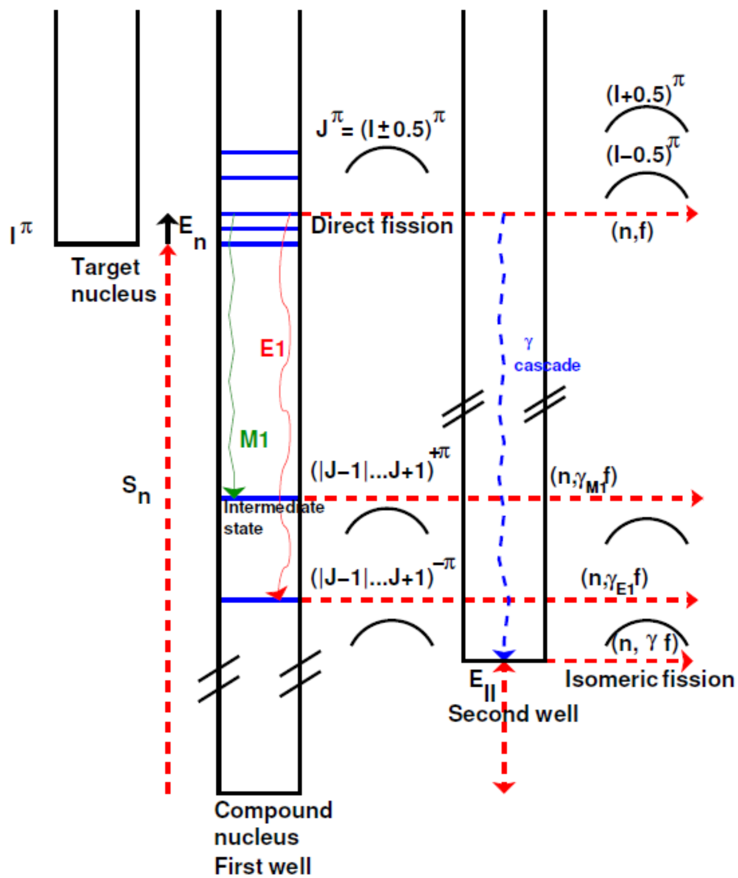
1967 : Evaluation des données neutroniques pour le Pu-239, G. LeCoq, PhD thesis

1973 : Etudes des sections efficaces de réaction des neutrons de resoanance avec Pu239, H. Derrien, PhD thesis

1974 : Etude des neutrons et des rayons gamma émis lors de la fission induite dans 235U et 239Pu par neutrons lents: mise en évidence de la réaction (n,γf), D. Shackleton, PhD thesis

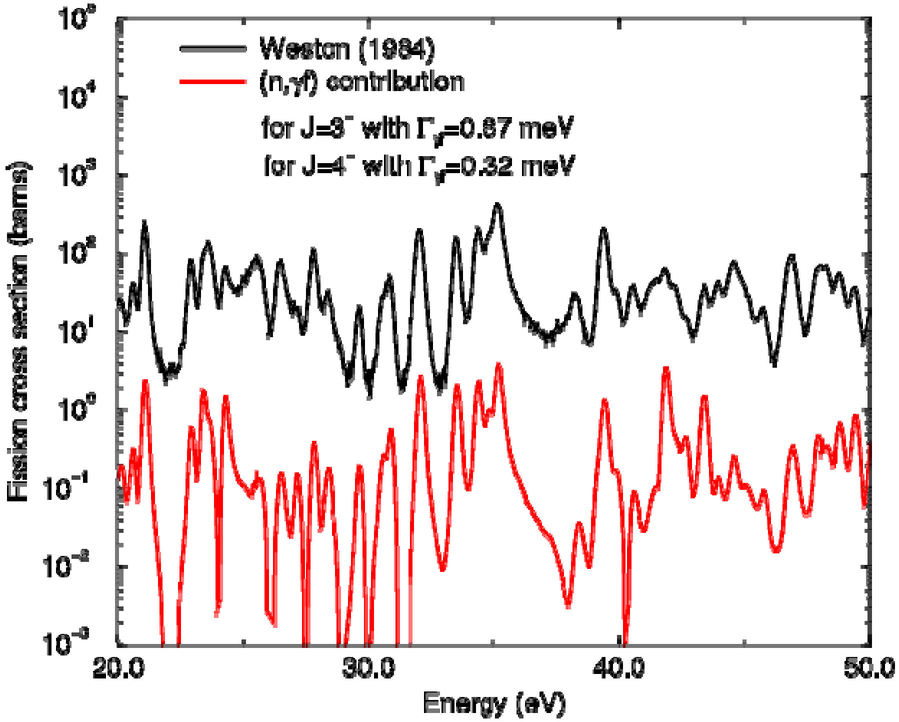
1980 : The double-humped fission barrier, S. Bjornholm and E. Lynn, Rev. Mod. Phys. 52

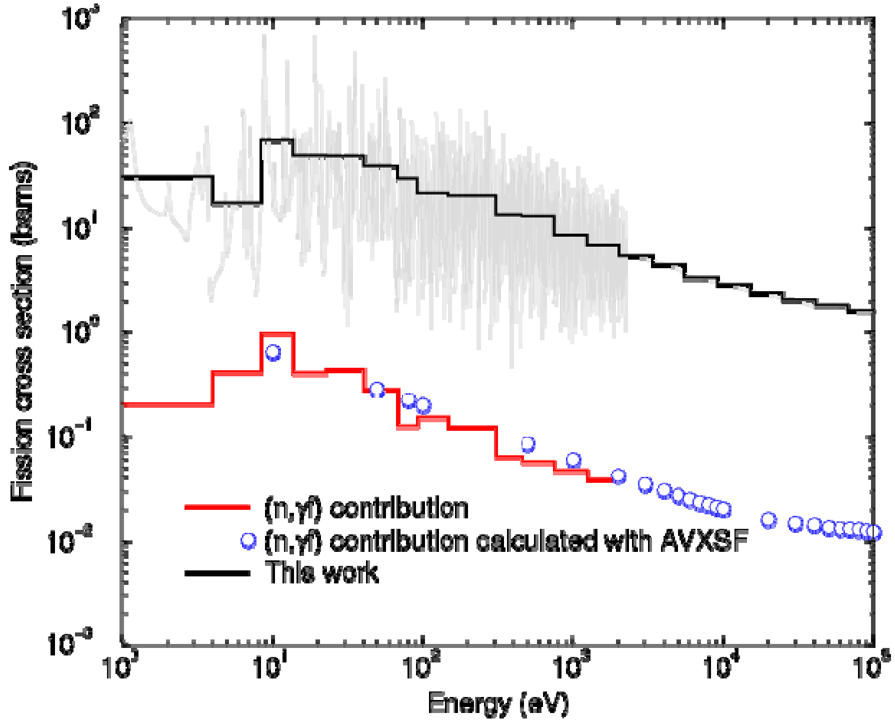
Two-step (n,f) processes in first and second well of fission barrier potential



Estimation of the (n,γf) reaction using the new U-235 resonance parameters

- Contribution close to 1%
- Good agreement with AVXSF calculations





⇒ how to include the (n,γf) widths in the Reich-Moore formalism ?

Conclusions

- ✓ Perform further benchmark testing;
- ✓ Temperature effects?
- ✓ Na-void reactivity of BFS and FCA;
- ✓ Revise the unresolved resonance region evaluation;
- ✓ High energy data? What is going on?
- ✓ Investigate other parameters such as PFNS and nubar: any need for improvements?
- ✓ How about fast systems?
- ✓ Continue work under the CIELO project;