Resonance Evaluation at ORNL

L. Leal (ORNL)

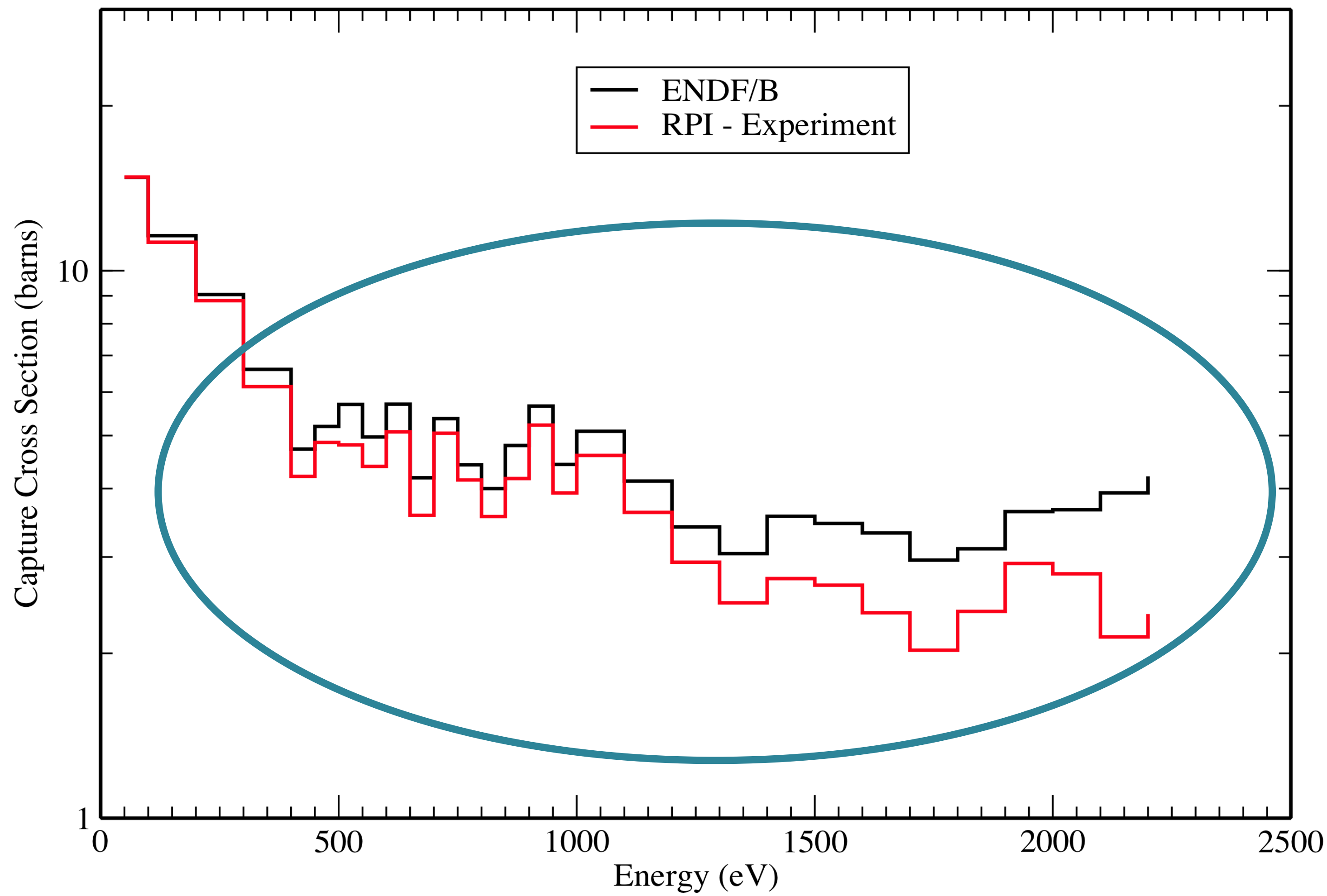
Y. Danon (RPI)

CSEWG, Nov 5-9, 2012

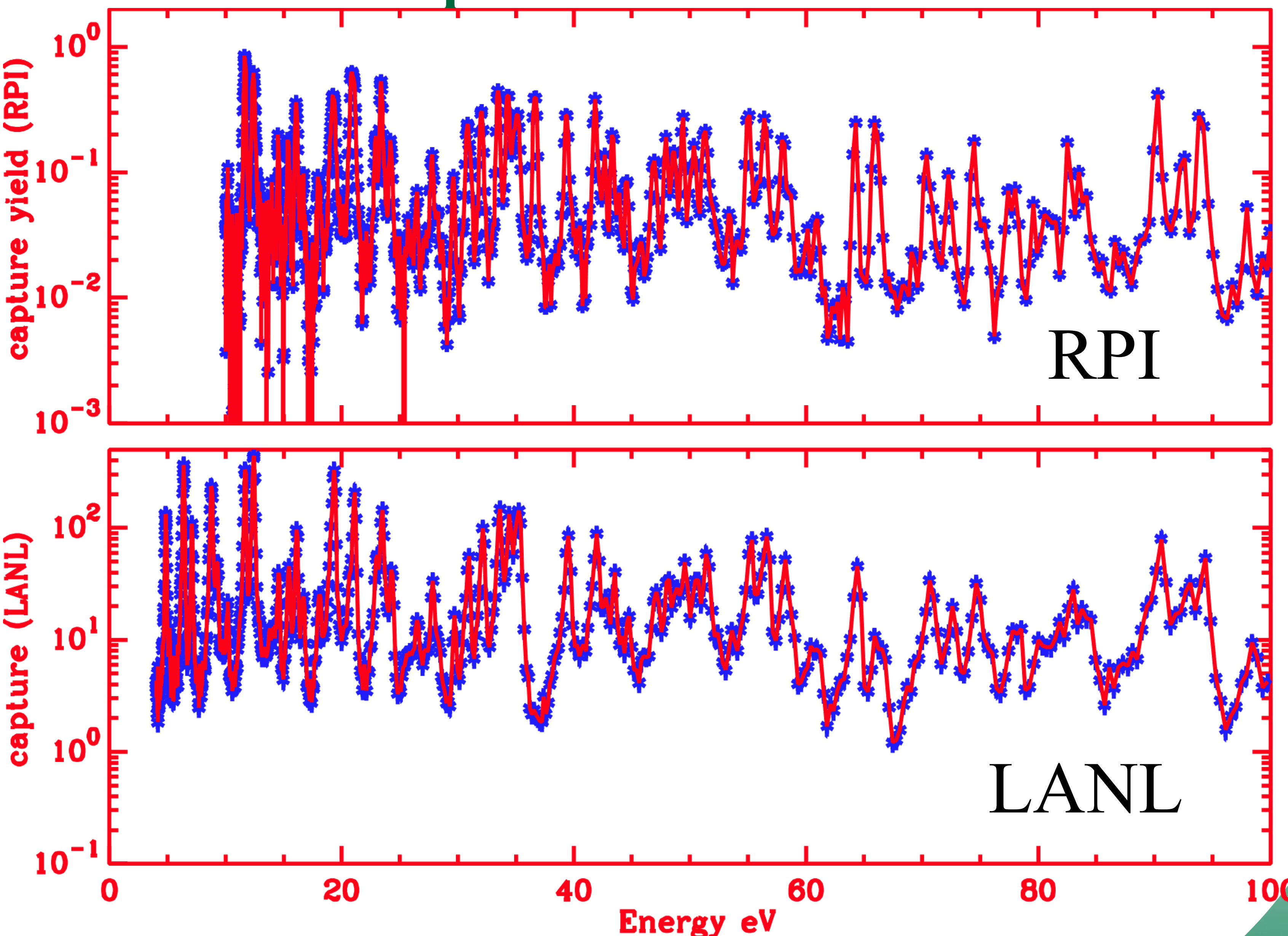
^{235}U Evaluation:

- ✓ **Intermediate energy benchmark problems;**
- ✓ **Fit new data measurements from RPI (capture and fission yields);**
- ✓ **Capture data from LANL;**
- ✓ **Test the new SAMMY ^{235}U evaluation in benchmark calculations: ZEUS benchmarks;**
- ✓ **Use JENDL4 as the template;**
- ✓ **Benchmark Calculations done with everything else from ENDF;**

RPI data and ENDF evaluation



RPI and LANL Capture Data



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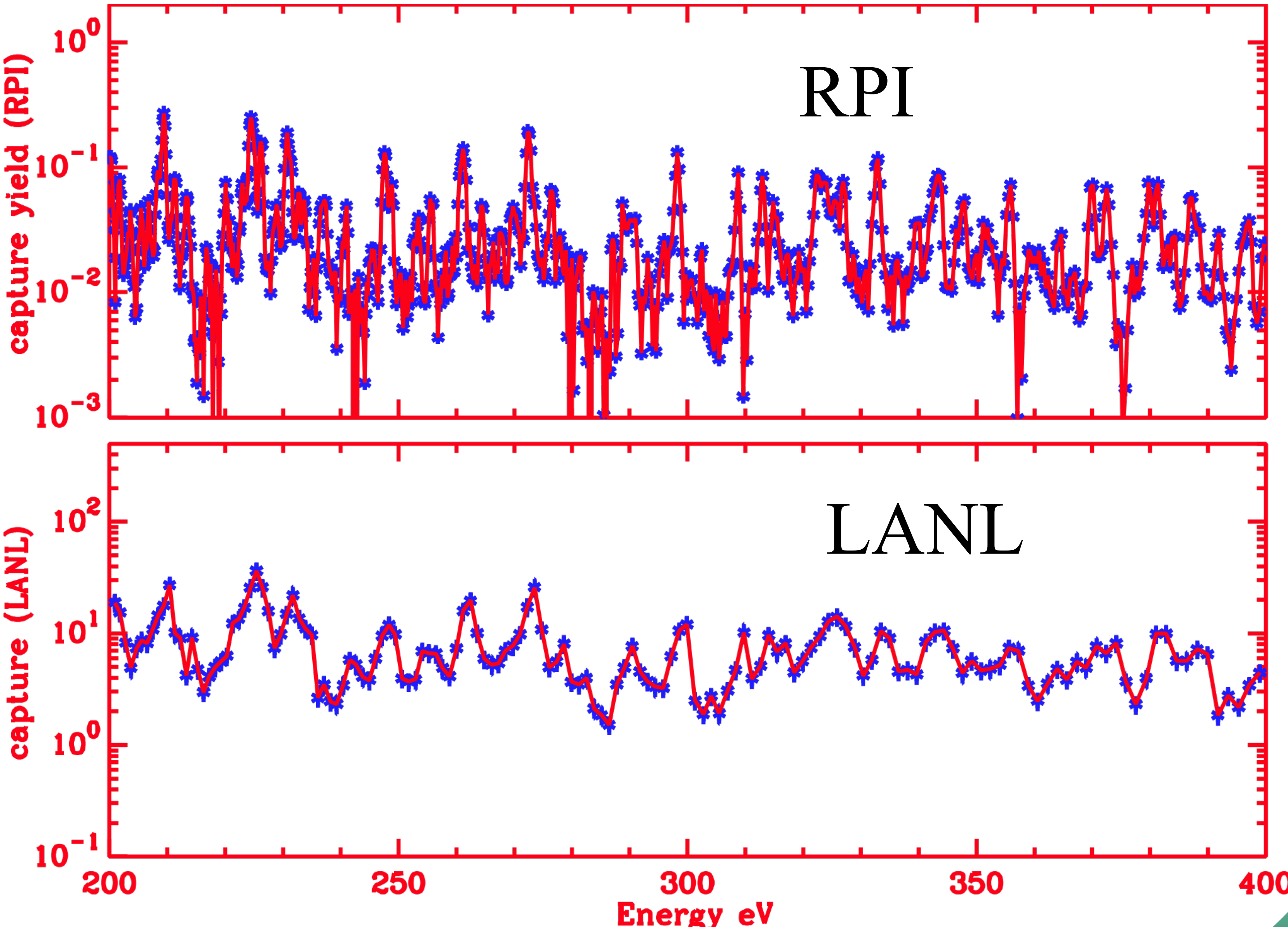
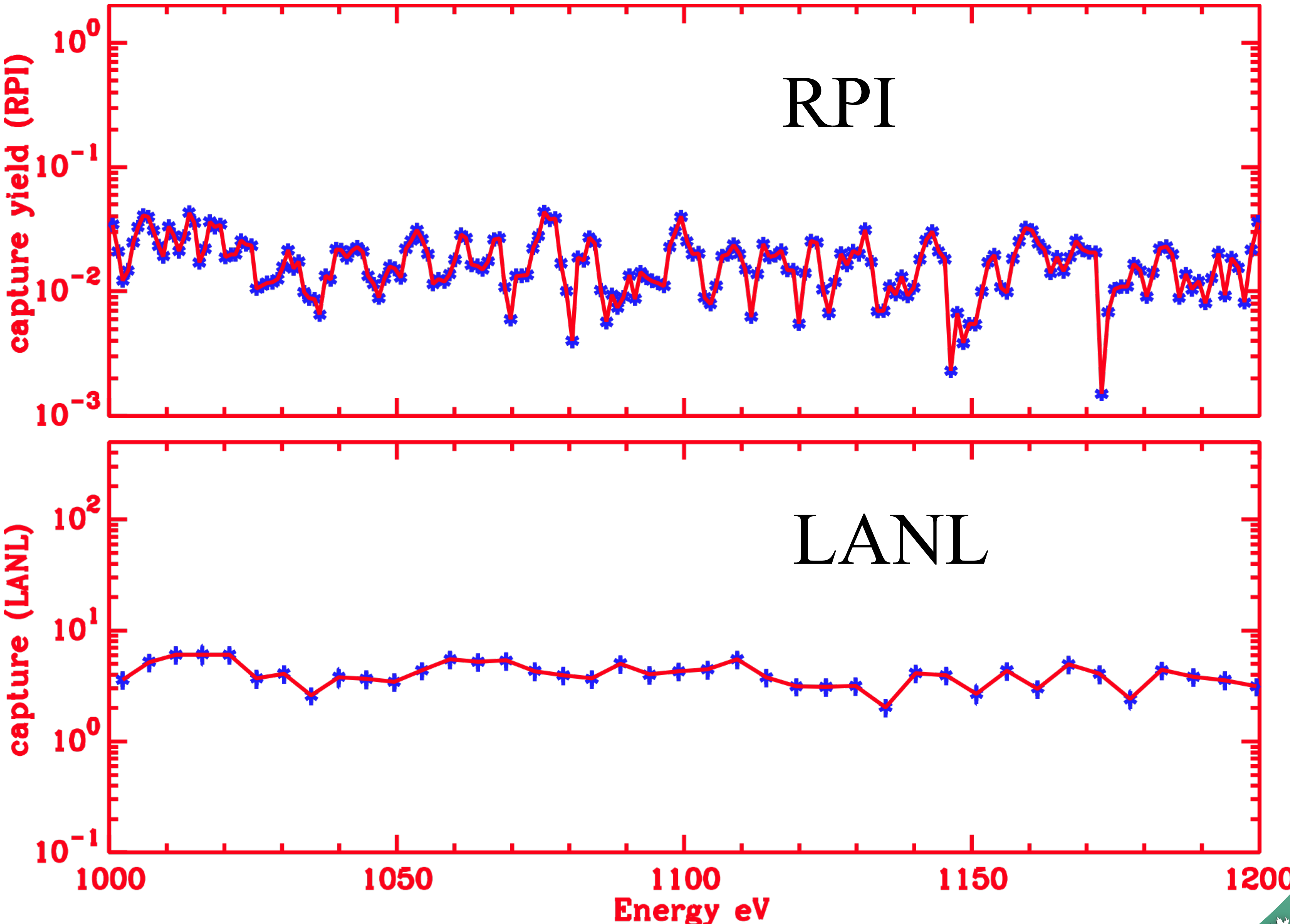
OAK RIDGE National Laboratory

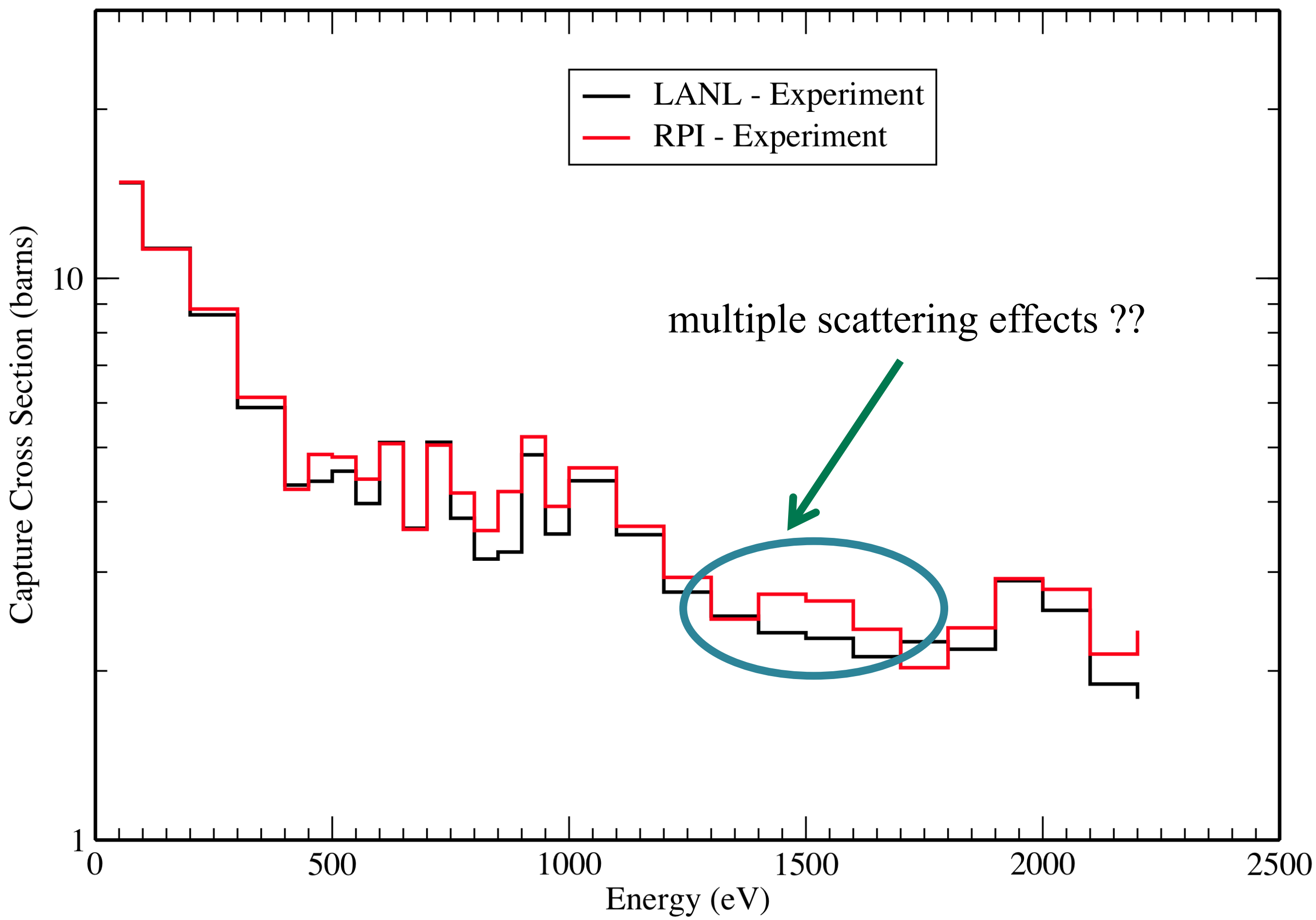
RPI and LANL Capture Data



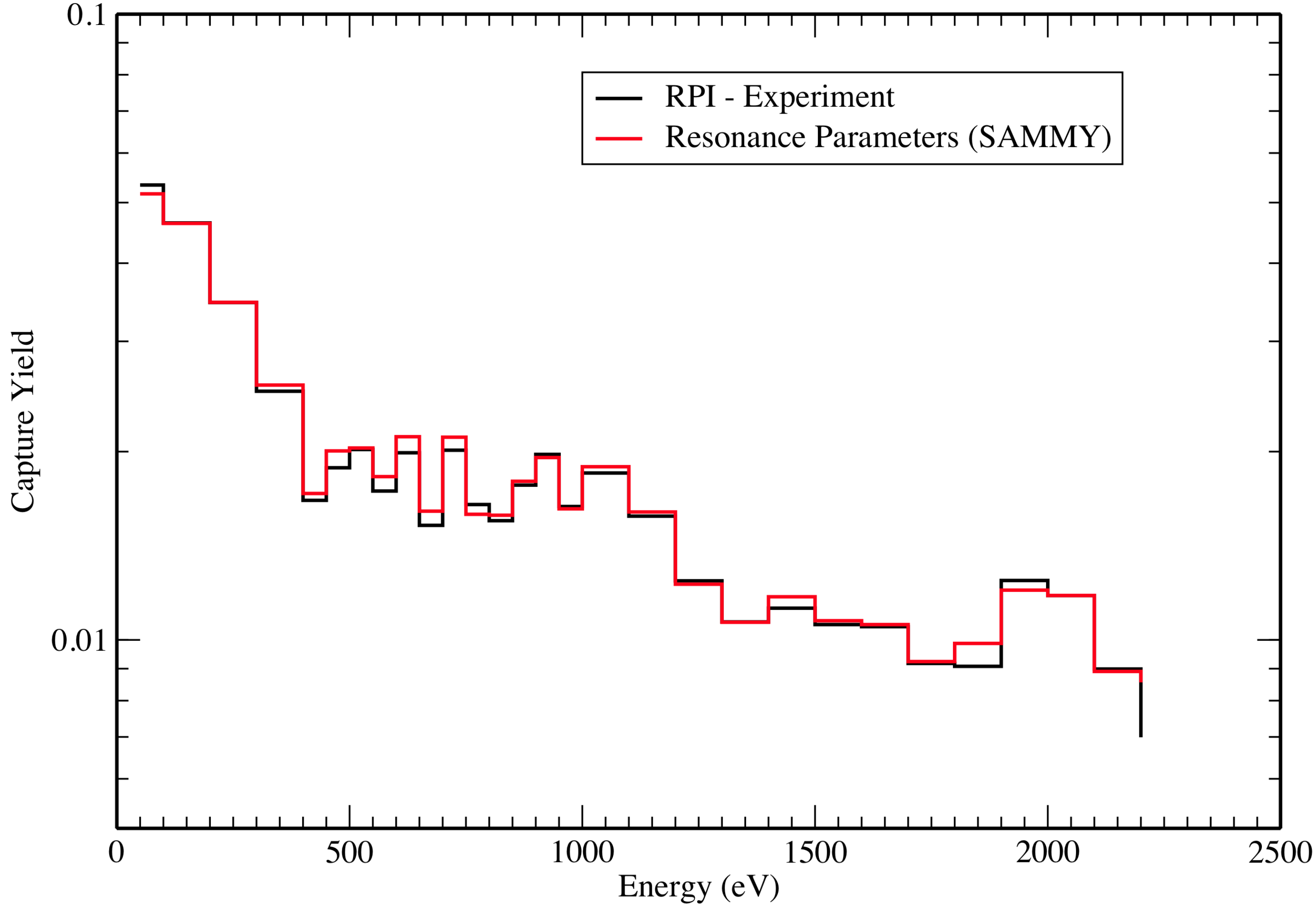
RPI and LANL Capture Data



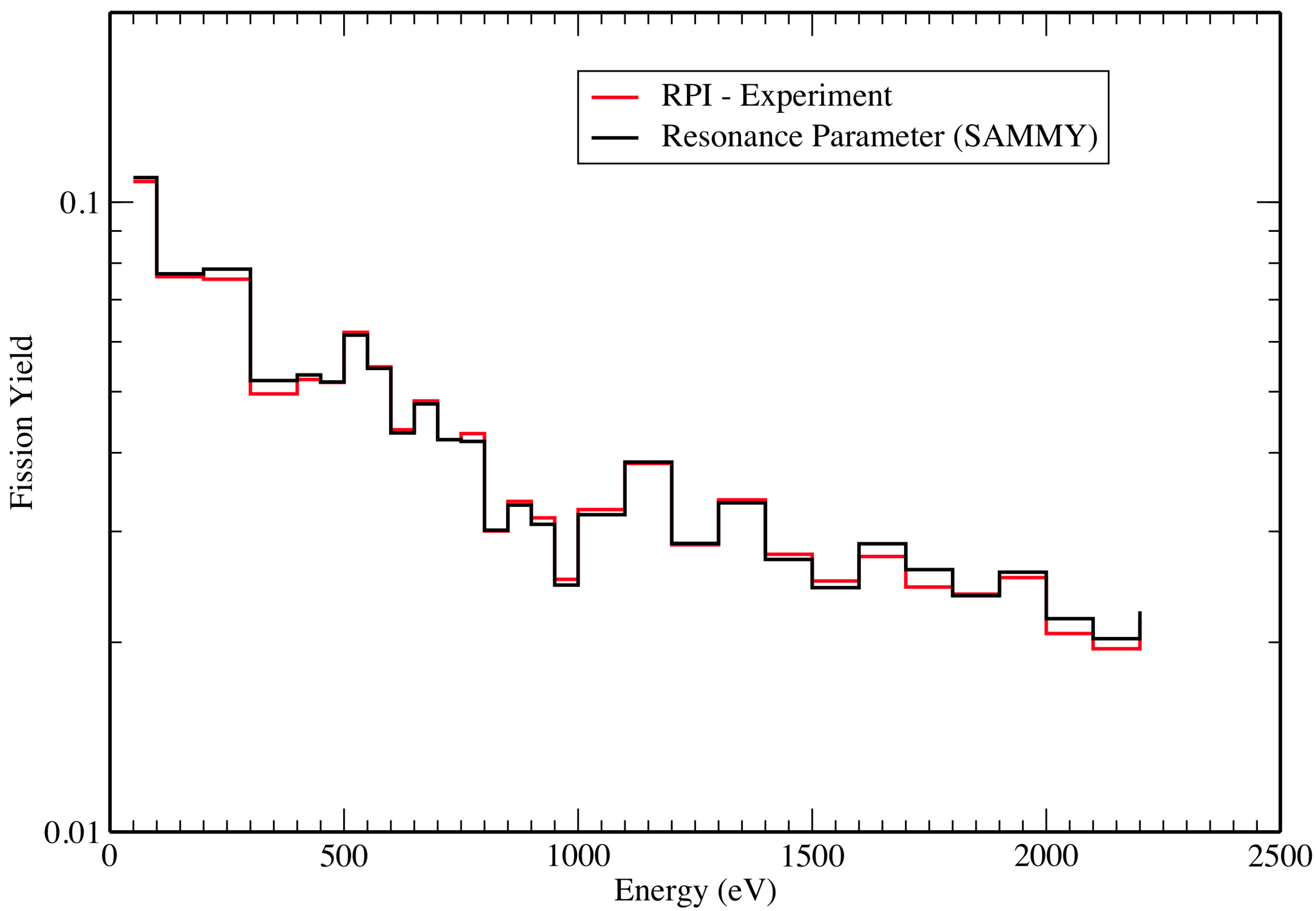
RPI and LANL Capture Data (average)



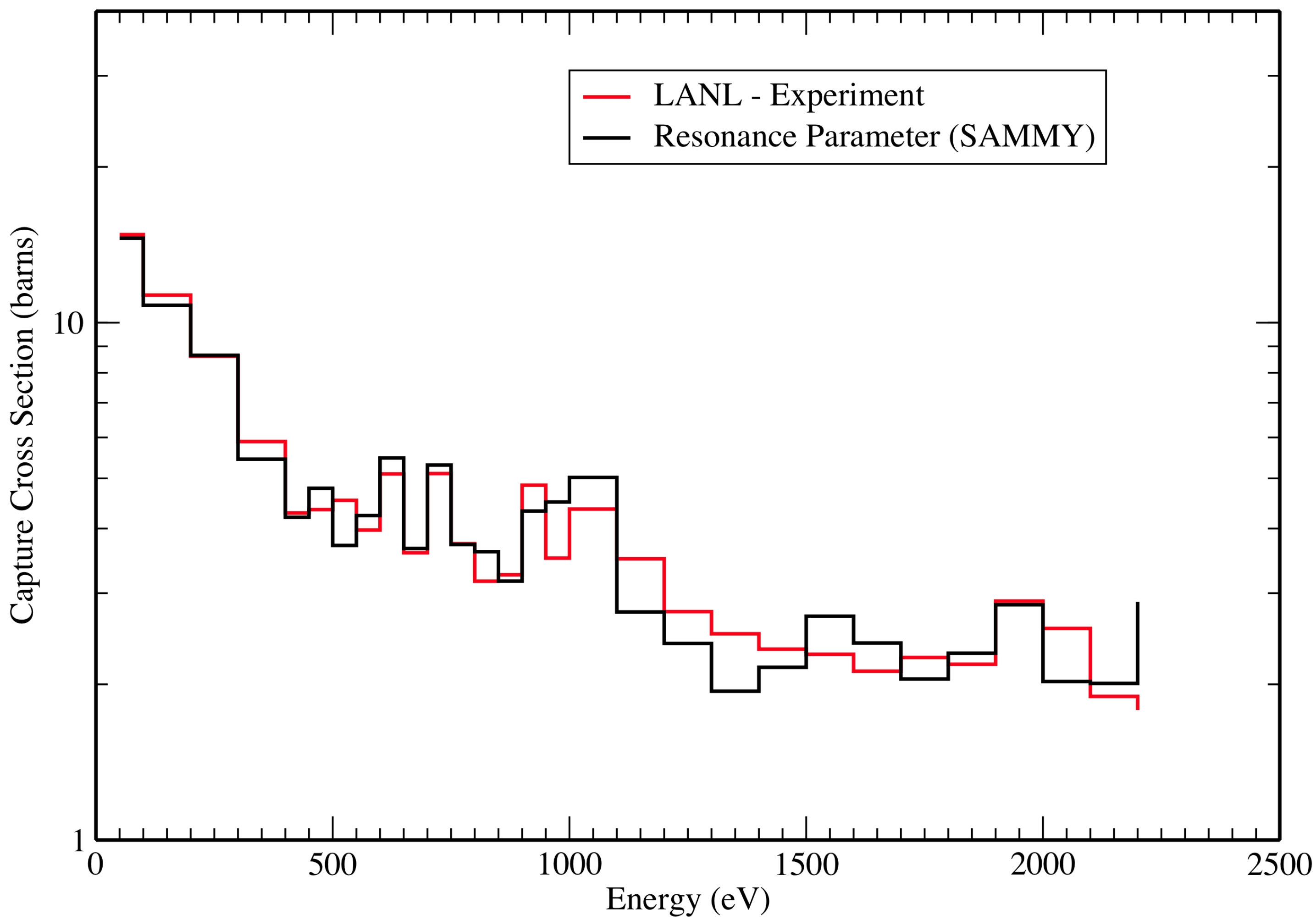
Fit of the RPI data



Fit of the RPI data



Fit of the LANL data



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

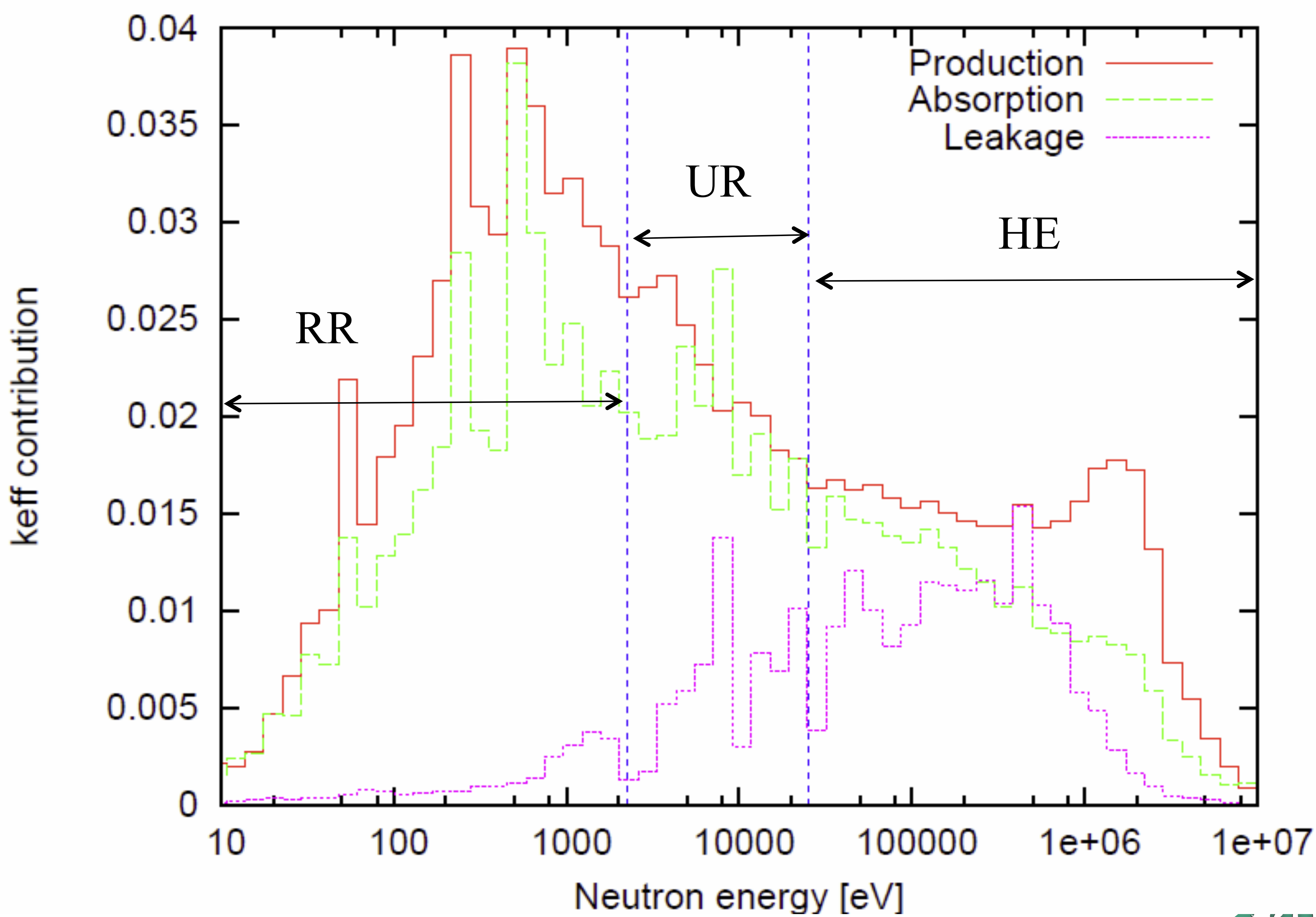
Case Number	k_{eff}	EALF (keV)	Intermediate-Energy Fission Fraction
1	0.9977 ± 0.0008	4.44	0.730
2	1.0001 ± 0.0008	9.45	0.698
3	1.0015 ± 0.0008	22.80	0.636
4	1.0016 ± 0.0008	80.80	0.503

EALF: Energy Average Lethargy Causing Fission

Effective System Multiplication Factor

$$k_{eff} = \frac{\Pr oduction}{Absorption + Leakage}$$

ZEUS1



0.04
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0.03
0.025
0.02
0.015
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1000
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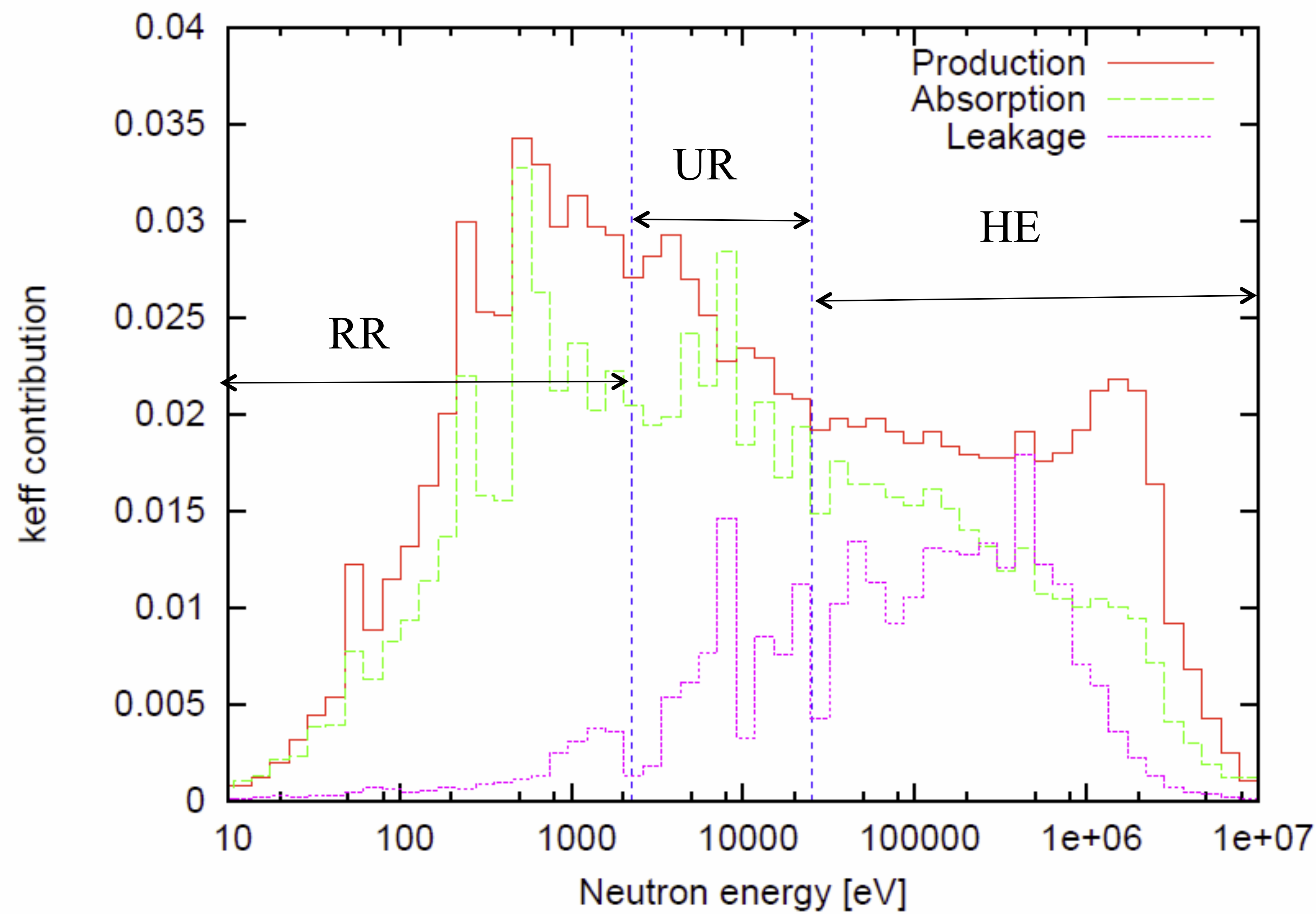
1e+06
1e+07
keff contribution
Neutron energy [eV]
Production
Absorption
Leakage
RR
UR
HE

ZEUS2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keff contribution
10
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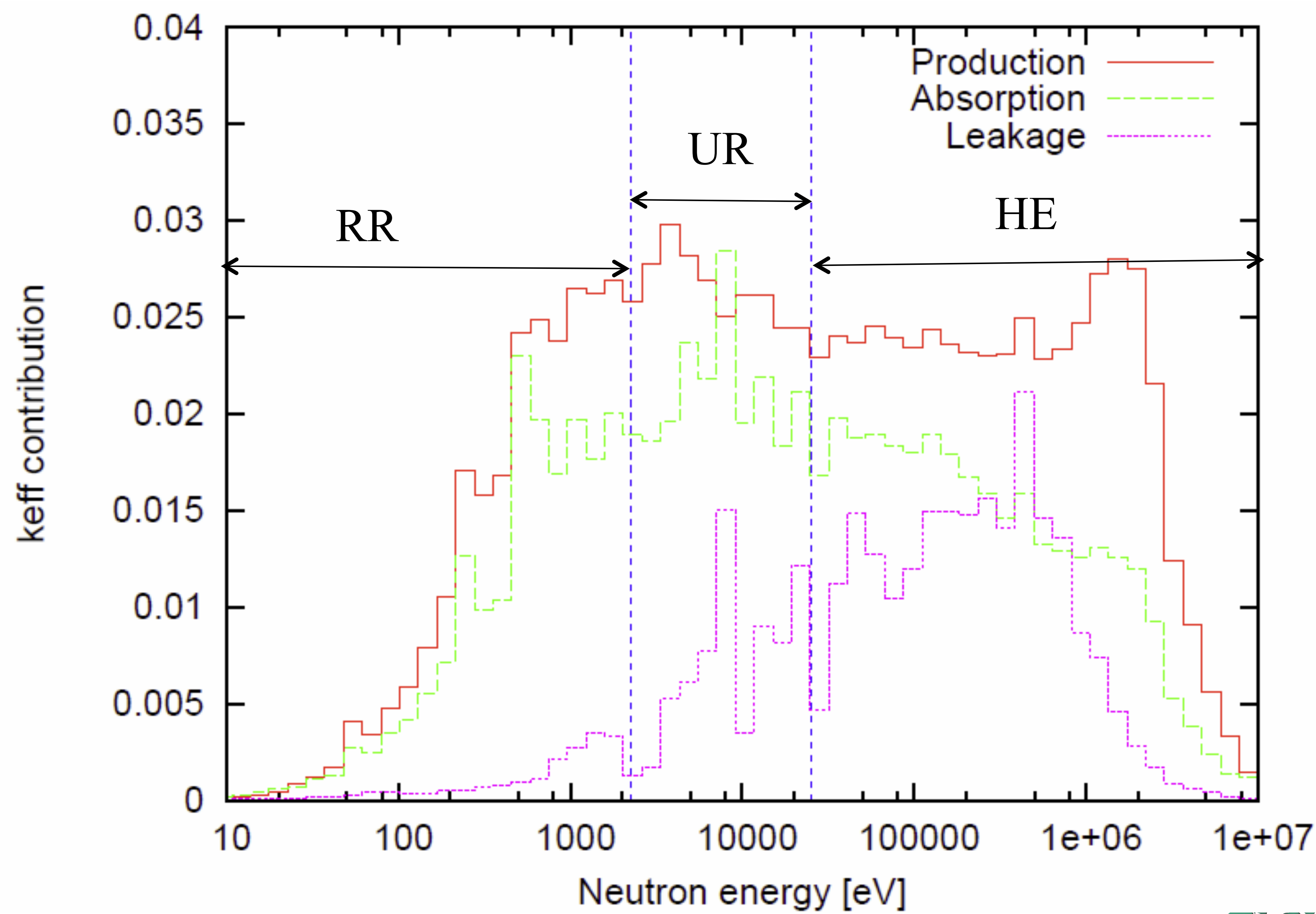
1e+06
1e+07
Neutron energy [eV]
Production
Absorption
Leakage
RR
UR
HE

ZEUS3



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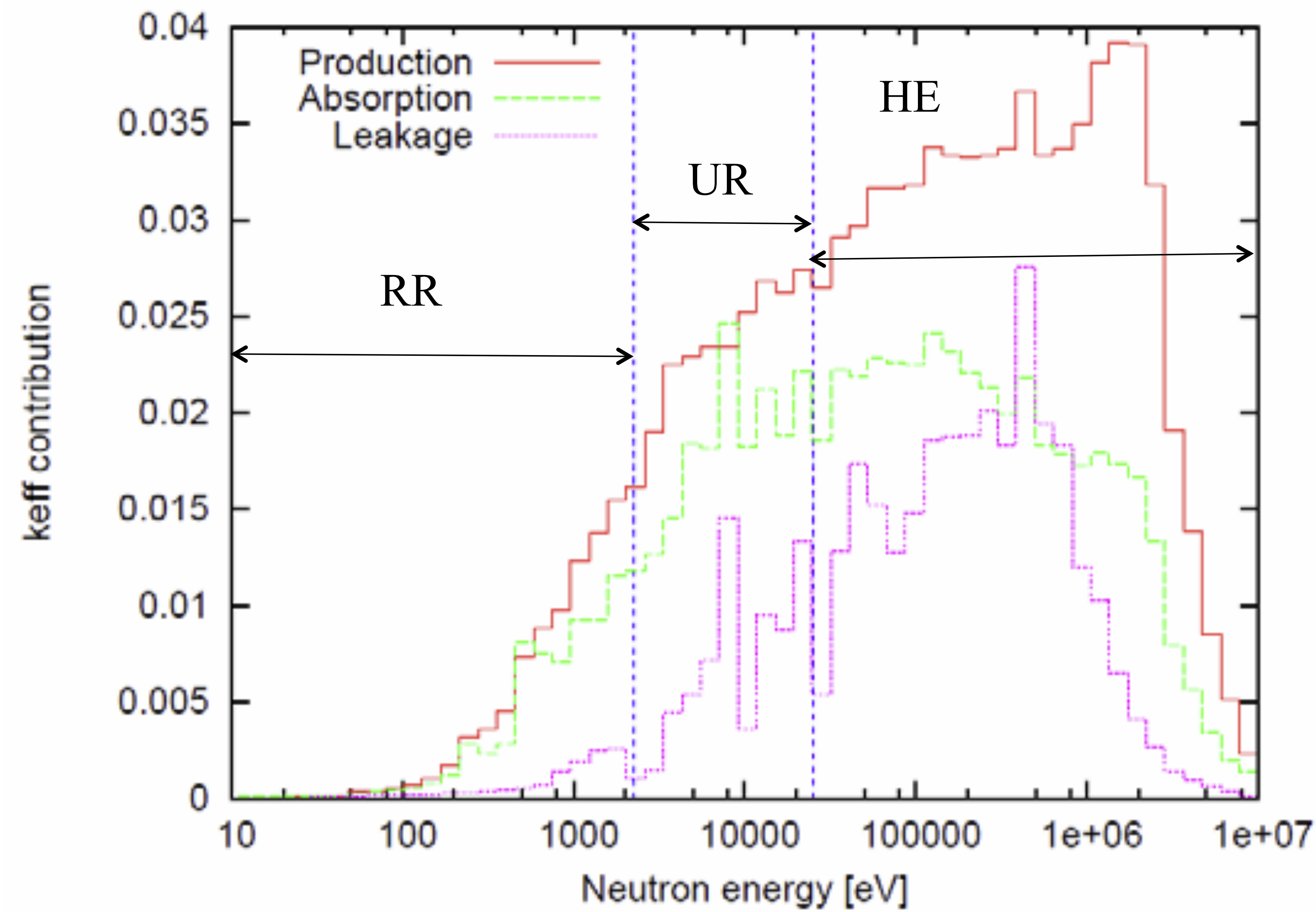
keff contribution
Neutron energy [eV]
Production
Absorption
Leakage
RR
UR
HE

ZEUS4

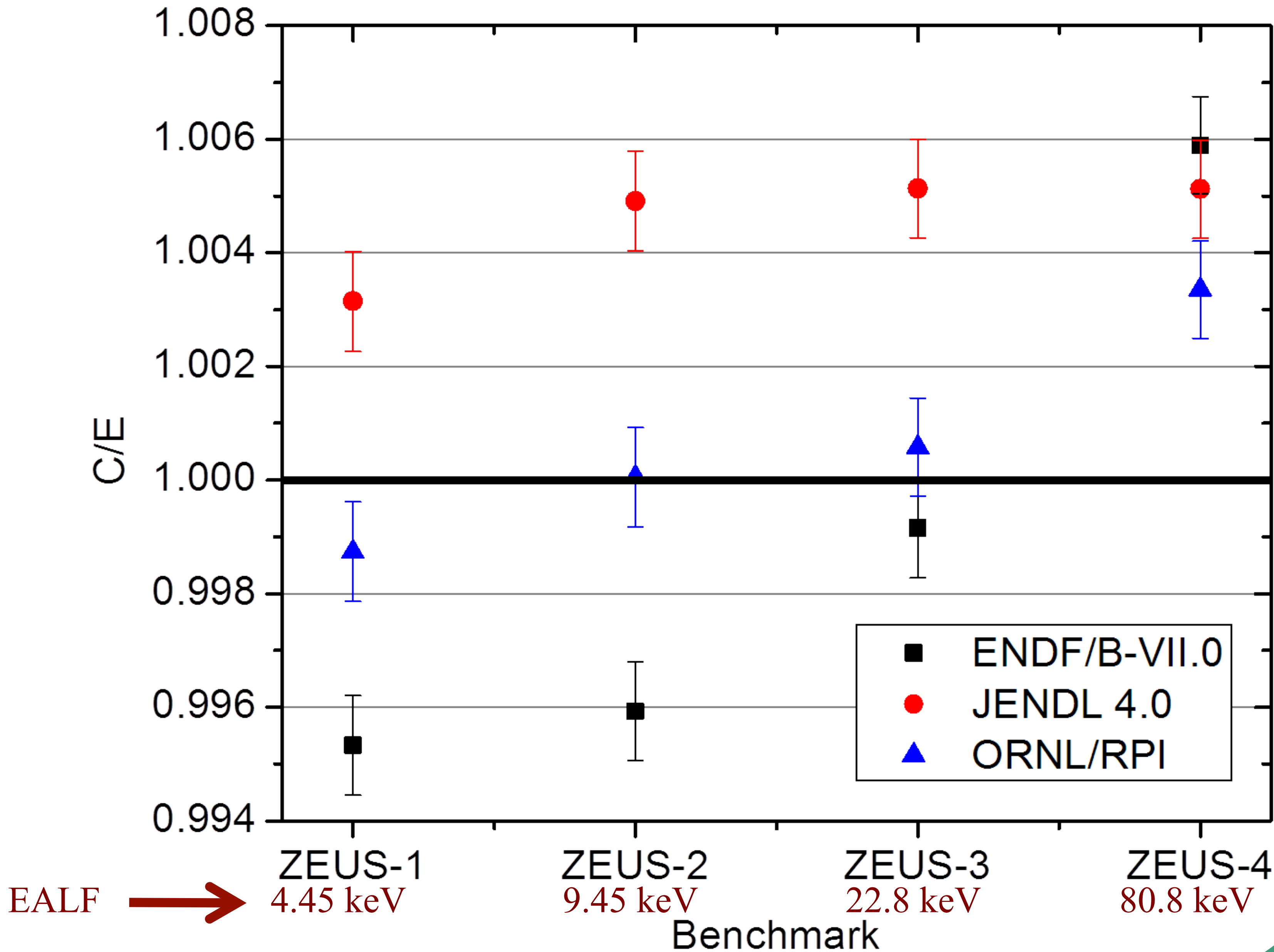


Production
Absorption
Leakage
HE
UR
RR
keff contribution
Neutron energy [eV]
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
10
100
1000
10000
100000
1e+06
1e+07

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)



Case Number	Benchmark Keff	Calculated keff			
		ENDF/B-VII.0	JENDL-4	JENDL4+ORNL	ENDF/B-VII.0+ORNL
HEU Benchmarks					
heu-met-fast-001 (godiva)	1.0000 ± 0.0010	0.99928 ± 0.00025	0.99751 ± 0.00026	0.99753 ± 0.00026	1.00004 ± 0.00027
heu-met-fast-028 (flattop)	1.0000 ± 0.0030	1.00320 ± 0.00030	0.99918 ± 0.00029	0.99886 ± 0.00029	1.00241 ± 0.00030
heu-met-inter-006-1 (ZEUS1)	0.9977 ± 0.0008	0.99304 ± 0.00035	1.00084 ± 0.00036	0.99644 ± 0.00035	1.00244 ± 0.00034
heu-met-inter-006-2 (ZEUS2)	1.0001 ± 0.0008	0.99603 ± 0.00035	1.00501 ± 0.00036	1.00015 ± 0.00035	1.00699 ± 0.00034
heu-met-inter-006-3 (ZEUS3)	1.0015 ± 0.0008	1.00065 ± 0.00035	1.00664 ± 0.00034	1.00208 ± 0.00033	1.00907 ± 0.00033
heu-met-inter-006-4 (ZEUS4)	1.0016 ± 0.0008	1.00750 ± 0.00031	1.00673 ± 0.00034	1.00496 ± 0.00031	1.01087 ± 0.00033
heu-sol-therm-013-case-1	1.0012 ± 0.0026	0.99848 ± 0.00026	0.99805 ± 0.00024	0.99771 ± 0.00024	0.99880 ± 0.00045
heu-sol-therm-013-case-2	1.0007 ± 0.0036	0.99745 ± 0.00026	0.99716 ± 0.00027	0.99690 ± 0.00028	0.99712 ± 0.00027
heu-sol-therm-013-case-3	1.0009 ± 0.0036	0.99417 ± 0.00028	0.99382 ± 0.00028	0.99327 ± 0.00028	0.99443 ± 0.00028
heu-sol-therm-013-case-4	1.0003 ± 0.0036	0.99571 ± 0.00030	0.99598 ± 0.00028	0.99501 ± 0.00029	0.99540 ± 0.00028
heu-sol-therm-032 (ORNL10-CSEWG)	1.0015 ± 0.0026	0.99906 ± 0.00017	0.99886 ± 0.00015	0.99894 ± 0.00017	0.99928 ± 0.00016

Case Number	Benchmark Keff	Calculated keff			
		ENDF/B-VII.0	JENDL-4	JENDL4+ORNL	ENDF/B-VII.0+ORNL
LEU Thermal Solution Benchmarks					
leu-sol-therm-002-case-1	1.0038 ± 0.0040	1.00002 ± 0.00025	0.99969 ± 0.00025	0.99905 ± 0.00025	1.00038 ± 0.00028
leu-sol-therm-002-case-2	1.0024 ± 0.0040	0.99594 ± 0.00028	0.99616 ± 0.00029	0.99618 ± 0.00028	0.99480 ± 0.00030
leu-sol-therm-007-case-14	0.9961 ± 0.0009	0.99495 ± 0.00030	0.99508 ± 0.00030	0.99487 ± 0.00031	0.99522 ± 0.00033
leu-sol-therm-007-case-30	0.9973 ± 0.0009	0.99771 ± 0.00031	0.99741 ± 0.00030	0.99744 ± 0.00031	0.99736 ± 0.00029
leu-sol-therm-007-case-32	0.9985 ± 0.0010	0.99579 ± 0.00029	0.99602 ± 0.00029	0.99589 ± 0.00031	0.99649 ± 0.00027
leu-sol-therm-007-case-36	0.9988 ± 0.0011	0.99860 ± 0.00027	0.99864 ± 0.00028	0.99830 ± 0.00028	0.99882 ± 0.00029
leu-sol-therm-007-case-49	0.9983 ± 0.0011	0.99752 ± 0.00028	0.99764 ± 0.00026	0.99716 ± 0.00025	0.99704 ± 0.00027

Case Number	Benchmark Keff	Calculated keff			
		ENDF/B-VII.0	JENDL-4	JENDL4+ORNL	ENDF/B-VII.0+ORNL
LEU Thermal Compound Benchmarks					
leu-com-therm-008-case-1	1.0007 ± 0.0016	1.00118 ± 0.00029	1.00136 ± 0.00029	0.99988 ± 0.00030	1.00134 ± 0.00031
leu-com-therm-008-case-2	1.0007 ± 0.0016	1.00131 ± 0.00030	1.00109 ± 0.00029	1.00036 ± 0.00030	1.00036 ± 0.00029
leu-com-therm-008-case-5	1.0007 ± 0.0016	1.00065 ± 0.00030	1.00064 ± 0.00029	0.99996 ± 0.00030	1.00000 ± 0.00031
leu-com-therm-008-case-7	1.0007 ± 0.0016	1.00029 ± 0.00030	1.00053 ± 0.00029	0.99971 ± 0.00030	1.00070 ± 0.00029
leu-com-therm-008-case-8	1.0007 ± 0.0016	1.00074 ± 0.00030	1.00014 ± 0.00029	0.99883 ± 0.00030	0.99991 ± 0.00030
leu-com-therm-008-case-11	1.0007 ± 0.0016	1.00203 ± 0.00030	1.00175 ± 0.00029	1.00044 ± 0.00030	0.99891 ± 0.00030

Resonance Evaluation at ORNL

L. Leal (ORNL)

CSEWG, Nov 5-9, 2012

Oak Ridge National Laboratory

^{239}Pu Resonance Evaluation
Presence of ^{239}Pu in a Nuclear System

- For a critical (or subcritical) nuclear system the fuel-temperature reactivity coefficient is negative. The presence of ^{239}Pu can make it positive;
- The ^{239}Pu resonance at ~ 0.3 eV produces fissions and some capture and therefore increases reactivity;
- As the ^{239}Pu builds up more fissions are produced leading to a change in the reactivity;
- Determination of the ^{239}Pu content in the spent fuel and an accurate knowledge of the nuclear data is needed for a safe shipping and cask design;

^{239}Pu Resonance Evaluation

Motivation:

- Existing resonance evaluation divided into three disjoint resonance parameter sets (computer limitations at the time ~ 1986) :

1.0×10^{-5} eV - 1 keV, 1 keV - 2 keV, 2 keV - 2.5 keV;

Issues are:

- Cross section mismatch at the energy boundaries;
- Not easy to generate uncertainty for the whole energy region (zero correlations between energy regions);
- Solve long standing problem for thermal benchmark;

Early Evaluation (Leal/Derrien at ORNL - 2008)

- One single set of resonance parameters covering the energy range:

  1.0×10^{-5} eV to 2.5 keV;

- Cross section mismatch at the energy boundaries gone!
- Uncertainty for the whole energy region generated with correlations properly determined!!
- Does it solve the problem of thermal benchmark?

Issues with ORNL Evaluation

- Results of plutonium solution calculations indicate no improvement using the new ORNL evaluation. Longstanding problem persists!!

- In some case the good results from previous ^{239}Pu evaluation deteriorated;

- Can the problem be solved?

- Efforts from ORNL, LANL and CEA (France)

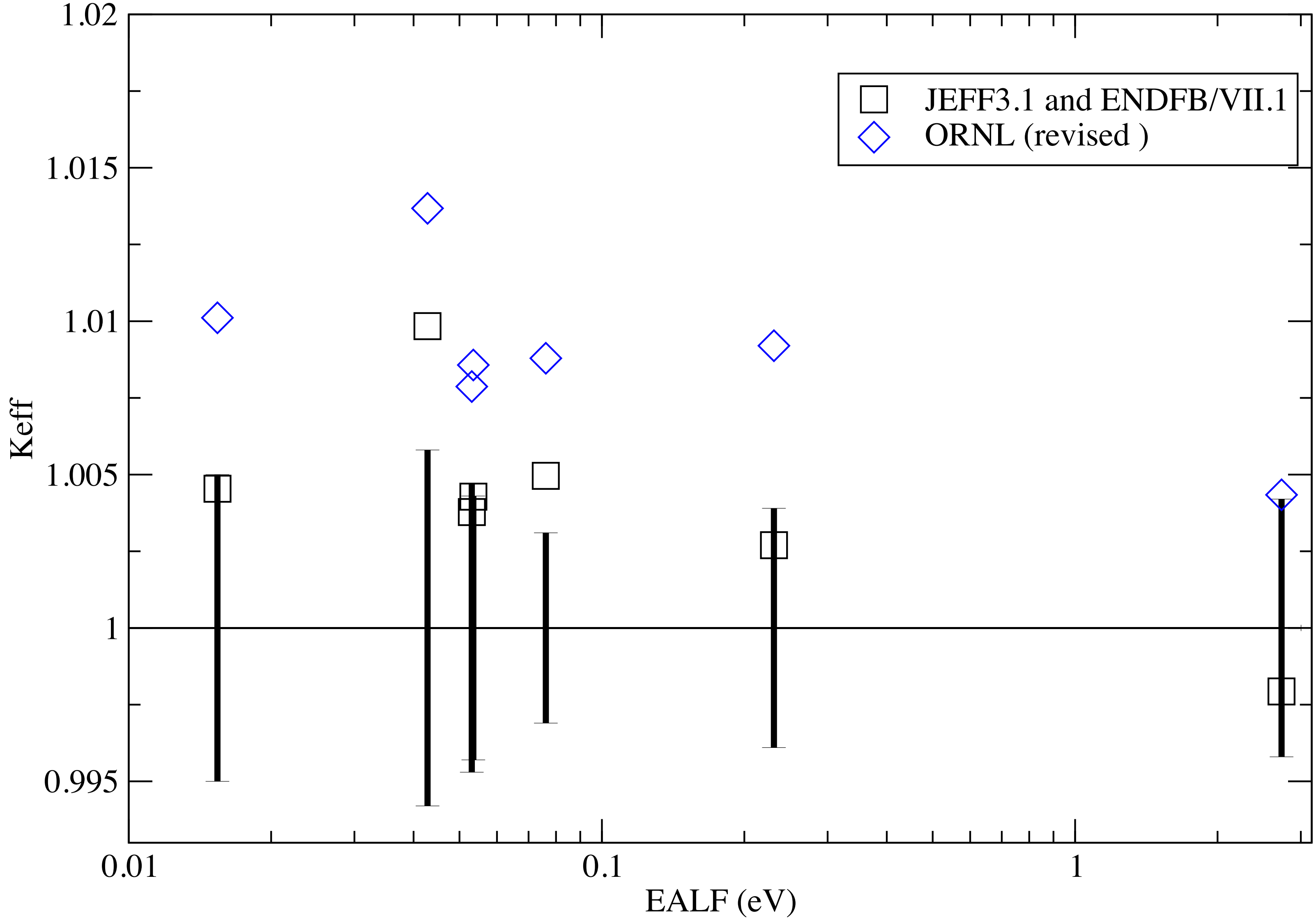
Integral Benchmark Experiments

- Benchmark from the ICSBEP;
- Plutonium Solution Systems;
- A good choice would be those benchmark experiments spanning the energy region from 0.01 eV to 3 eV
- Choice based on the Energy of Average Lethargy Causing Fission (EALF)

Benchmark problem from ICSBEP

Benchmark	Experimental *Keff*	EALF(eV)	
PST1.4	1.0000 ± 0.0050	0.0154	5 % ^{240}Pu
PST4.1 (sphere)	1.0000 ± 0.0047	0.0531	5 % ^{240}Pu
PST12.10 (cubic tank)	1.0000 ± 0.0047	0.0535	25 % ^{240}Pu
PST12.13	1.0000 ± 0.0047	0.0428	19 % ^{240}Pu
PST18.1 (cylinder)	1.0000 ± 0.0047	0.0761	43 % ^{240}Pu
PST34.4 (cylinder)	1.0000 ± 0.0047	0.231	116g Pu/L, 1.42g Gd/L
PST34.15	1.0000 ± 0.0047	2.730	363 g Pu/L, 20.25g Gd/L

EALF: Energy Average Lethargy Causing Fission



1.02
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Keff
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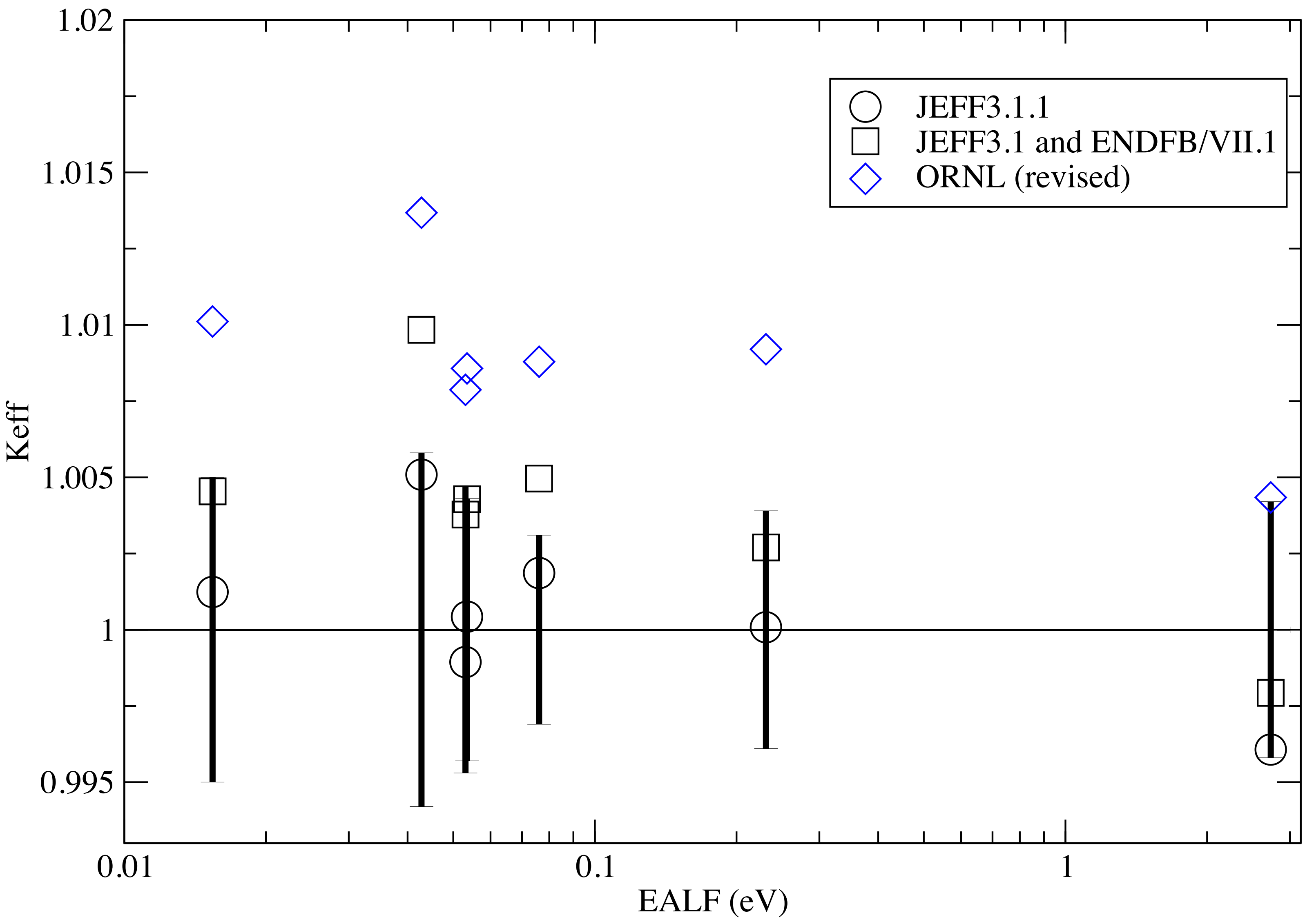
1
EALF (eV)
JEFF3.1 and ENDFB/VII.1
ORNL (revised)

JEFF3.1.1 Evaluation
(work done at French Atomic Commission/Cadarache)

- Improves substantially prediction of thermal critical systems multiplication factor - k_{eff};
- Work started based on the JEFF3.1 (ENDF/VII.1), that is, the three disjoint sets of resonance parameters;
- Some adjustments to other quantities such as nu-bar;
- Experimental cross section not well represented;



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EALF (eV)
JEFF3.1.1
JEFF3.1 and ENDFB/VII.1
ORNL (revised)

ORNL (USA) and Cadarache (France)

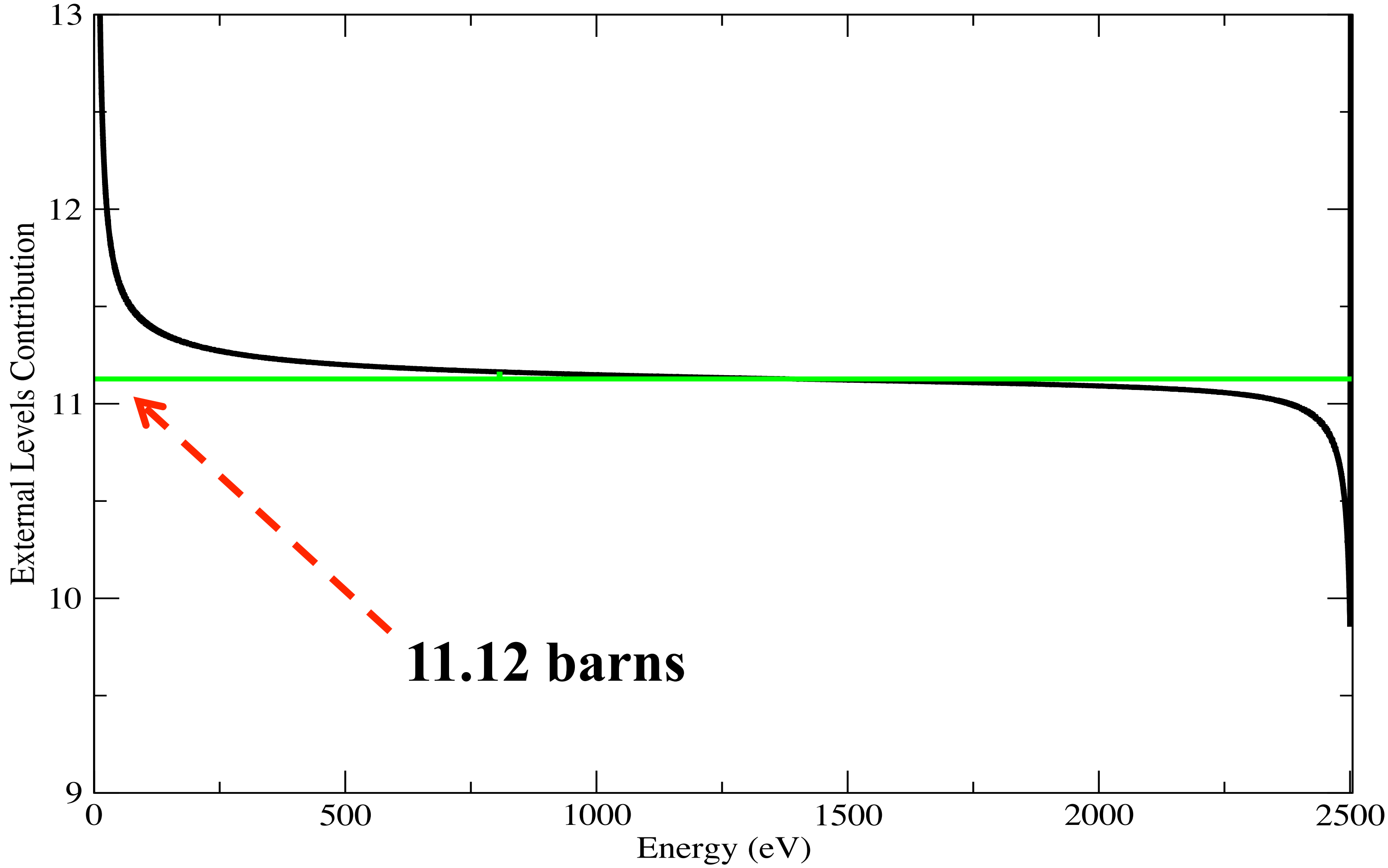
Work Strategy

- **Use the SAMMY code to perform resonance analysis using the best selected set of experimental time-of-flight data;**
- **Generate cross-section library with the NJOY code for use in benchmark calculations with the MCNP code;**
- **Generate cross-section library with the GALLILE (NJOY +CALENDF) code for use in benchmark calculations with the MCNP (USA), TRIPOLI and APOLLO French codes;**
- **Use a selected set of experimental benchmarks with average of neutron lethargy causing fission spanning the energy range from 0.01 eV to 3 eV;**
- **Use other benchmarks in addition to the ICSBEP. Examples are the MISTRAL and FUBILA experiments (MOX fuel) performed at the EOLE facility to test the evaluation in France;**

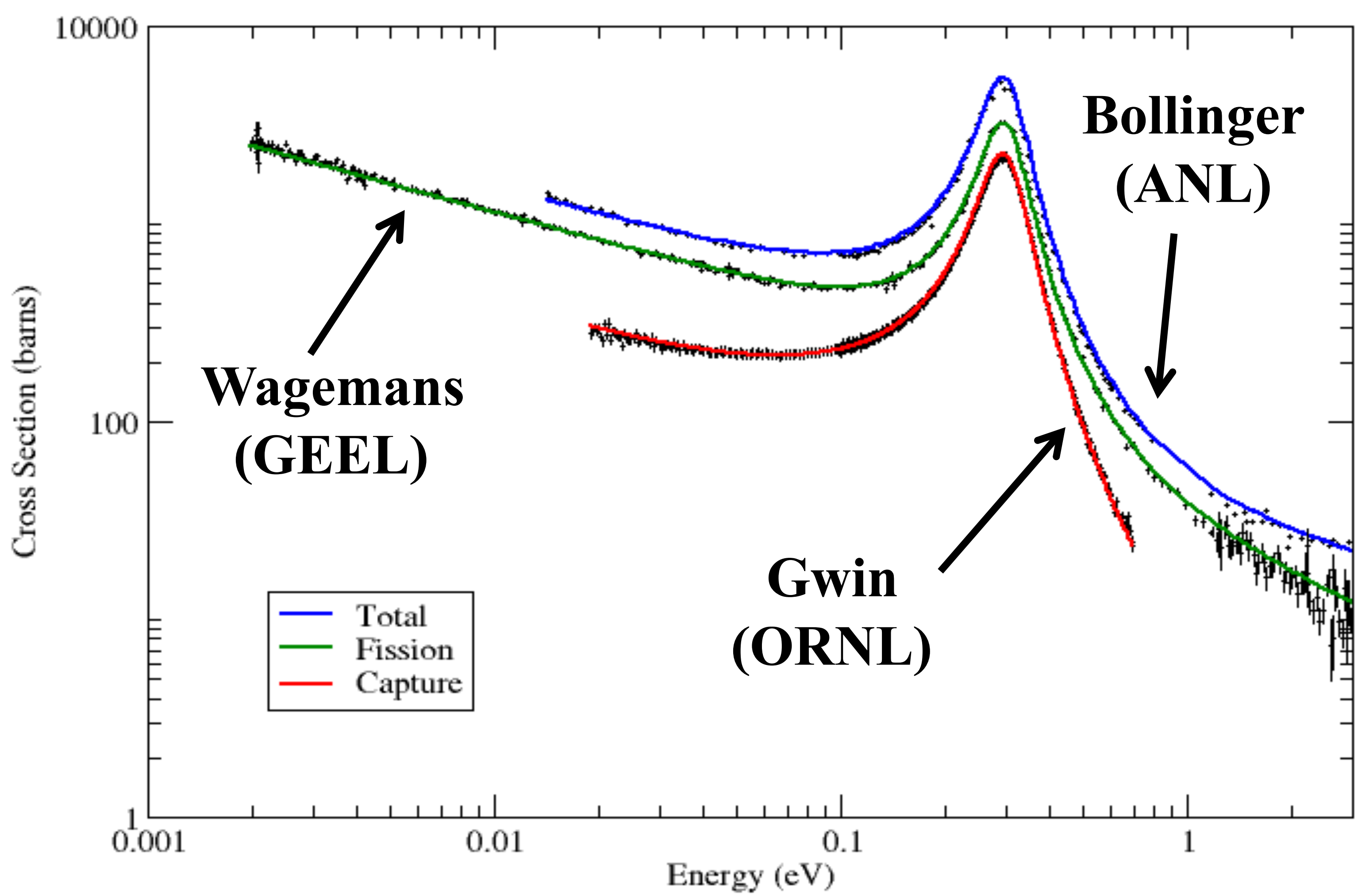
EXPERIMENTAL DIFFERENTIAL DATA

Reference	Energy Range (eV)	Facility	Measurement
Bollinger et al. (1956)	0.01 – 1.0	Chopper	Total Cross Section
Gwin et al. (1971)	0.01 – 0.5	ORELA	Fission and Absorption at 25.6 m
Gwin et al. (1976)	1.0 – 100.0	ORELA	Fission and Absorption at 40.0 m
Gwin et al. (1984)	0.01 – 20.0	ORELA	Fission at 8 m
Weston et al. (1984)	9.0 – 2500.0	ORELA	Fission at 18.9 m
Weston et al. (1988)	100.0 – 2500.0	ORELA	Fission at 86 m
Weston et al. (1993)	0.02 – 40.0	ORELA	Fission at 18.9 m
Wagemans et al. (1988)	0.002 – 20.0	GELINA	Fission at 8 m
Wagemans et al. (1993)	0.01 – 1000.0	GELINA	Fission at 8 m
Harvey et al. (1985)	0.7 – 30.0	ORELA	Transmission at 18 m
Harvey et al. (1985)	30.0 – 2500.0	ORELA	Transmission at 80 m

External Levels Determination



Cross Section Fitting



Integral Quantities:

- ✓ Benchmark experiments sensitive to the fission and capture cross sections, and also to nu-bar

- ✓ A right combination of capture, fission, and nub-bar may lead to an improvement on the k_{eff};

Eta and K1 are two important quantities in reactor calculations:

- ✓ Eta(***η***): six factor form
- ✓ K1: from first-order perturbation theory

Multiplication Factor: k_∞

$$Leakage \longrightarrow 0$$

$$\frac{\text{Pr}\,oduction}{Absorption}$$

$$k_\infty \propto \eta = \frac{\nu \sigma_f}{\sigma_a}$$

K1 Factor: first-order perturbation theory

Reactivity change: $\delta\rho$

$$\delta\rho = \frac{<\phi^{+}, \Delta H \phi>}{<\phi^{+}, P\phi>}$$

$$\Delta H = \mathrm{Pr}\,oduction - Absorption$$

Equivalent K1

$$K1 = \nu\sigma_f - \sigma_a$$

$$\eta = \frac{\nu\sigma_f}{\sigma_a}$$

and

$$K1 = \nu\sigma_f - \sigma_a$$

Benchmarks sensitive to K1, i.e., the difference:

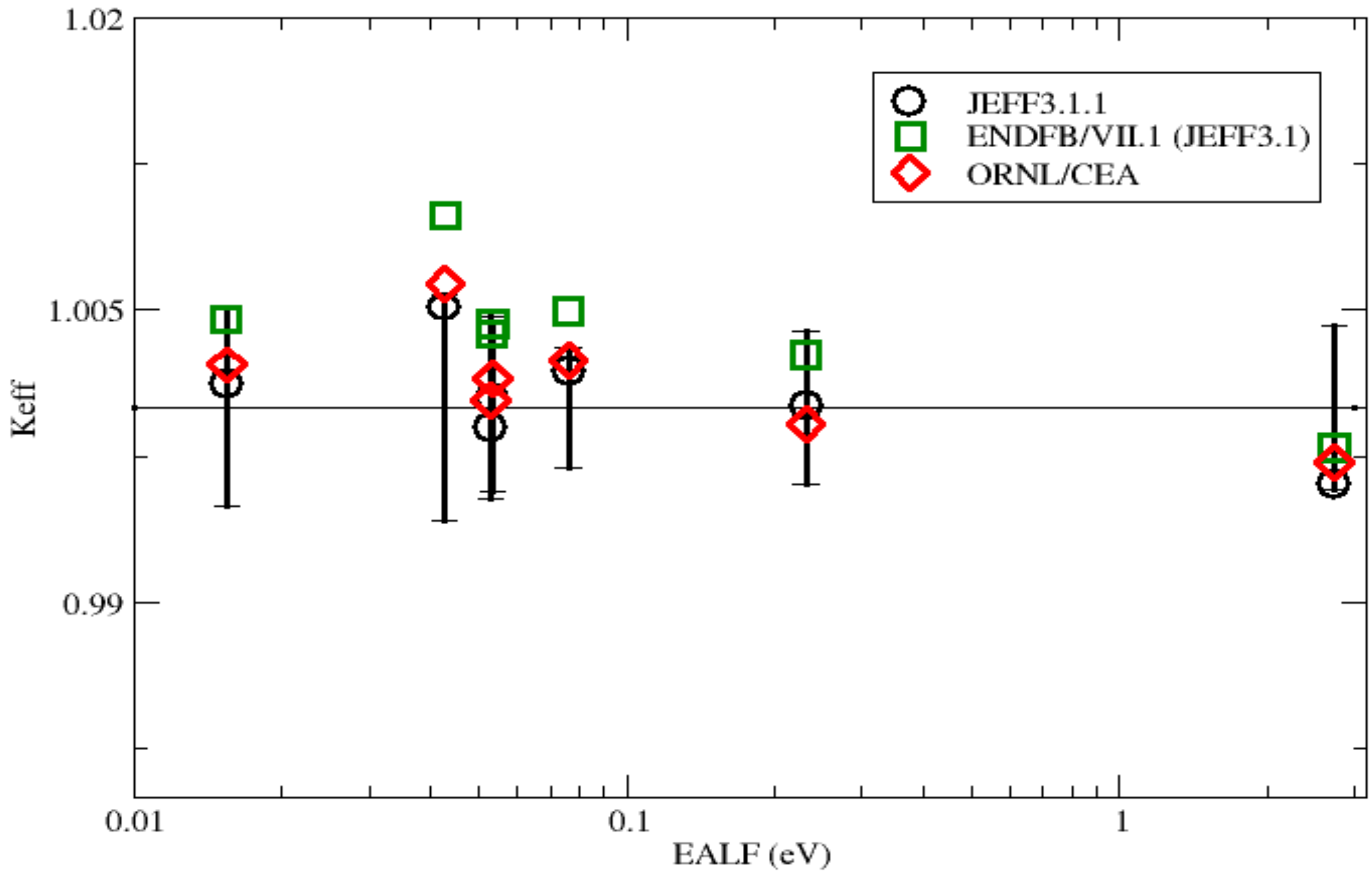
production - absorption

Thermal values and integral quantities calculated with SAMMY

Quantity	ANR	ENDF/B-VII.1 (JEFF3.1)	JEFF3.1.1	NEW (ORNL/CEA)
σ_γ	269.3 ± 2.9	270.64	272.72	270.06
σ_f	748.1 ± 2.0	747.65	747.08	747.19
g_f	1.0553 ± 0.0013	1.0544	1.0495	1.0516
g_a	1.0770 ± 0.0030	1.0784	1.0750	1.0771
$\bar{\nu}$	2.879 ± 0.006	2.873	2.873	2.873
I_γ	180 ± 20	181.44	181.50	180.09
I_f	303 ± 10	302.60	303.58	309.09
$K1$	1177.25	1166.62	1156.35	1161.30

ANR: Atlas of Neutron Resonance

ICSBEP Benchmark Results (everything else from BVII.1)



ORNL Resonance Evaluations and deliverables

	Energy Range	Resonance Covariance Evaluation	Target date for delivery the evaluation
^{63}Cu	Thermal to 300 keV	Yes	July FY2014
^{65}Cu	Thermal to 300 keV	Yes	July FY2014
^{182}W	Thermal to 10 keV	Yes	FY2014
^{183}W	Thermal to 5 keV	Yes	FY2014
^{184}W	Thermal to 10 keV	Yes	FY2014
^{186}W	Thermal to 10 keV	Yes	FY2014
^{56}Fe	Thermal to 2 MeV	Yes	FY2014
^{239}Pu	Thermal to 2.5 keV	Use ENDF/B-VII.1 (FILE33)	FY2012
^{235}U	Thermal to 2.25 keV	Use ENDF/B-VII.1 (FILE33)	FY2013