

Validation Study on G-versions of U-238 Evaluations for JEFF

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I. Introduction



Update of U-238 Reaction Cross Sections

- ◆ An effort has been devoted to the update in the resonance energy region
 - ☞ under the JEFF project
 - ☞ further consideration in both CIELO Pilot Project and Neutron Cross-Section Standards Project by IAEA
- ◆ G-versions of U-238
 - ☞ new evaluations by I. Sirakov in 2014
 - ☞ required for an extensive validation test



◆ Validation study on G-versions of U-238

- ☞ 94 criticality benchmark problems taken from expanded criticality validation suite for MCNP
- ☞ Overall performances of G-versions
- ☞ Influence due to extension of energy boundary between RR and URR

II. G-versions of U-238



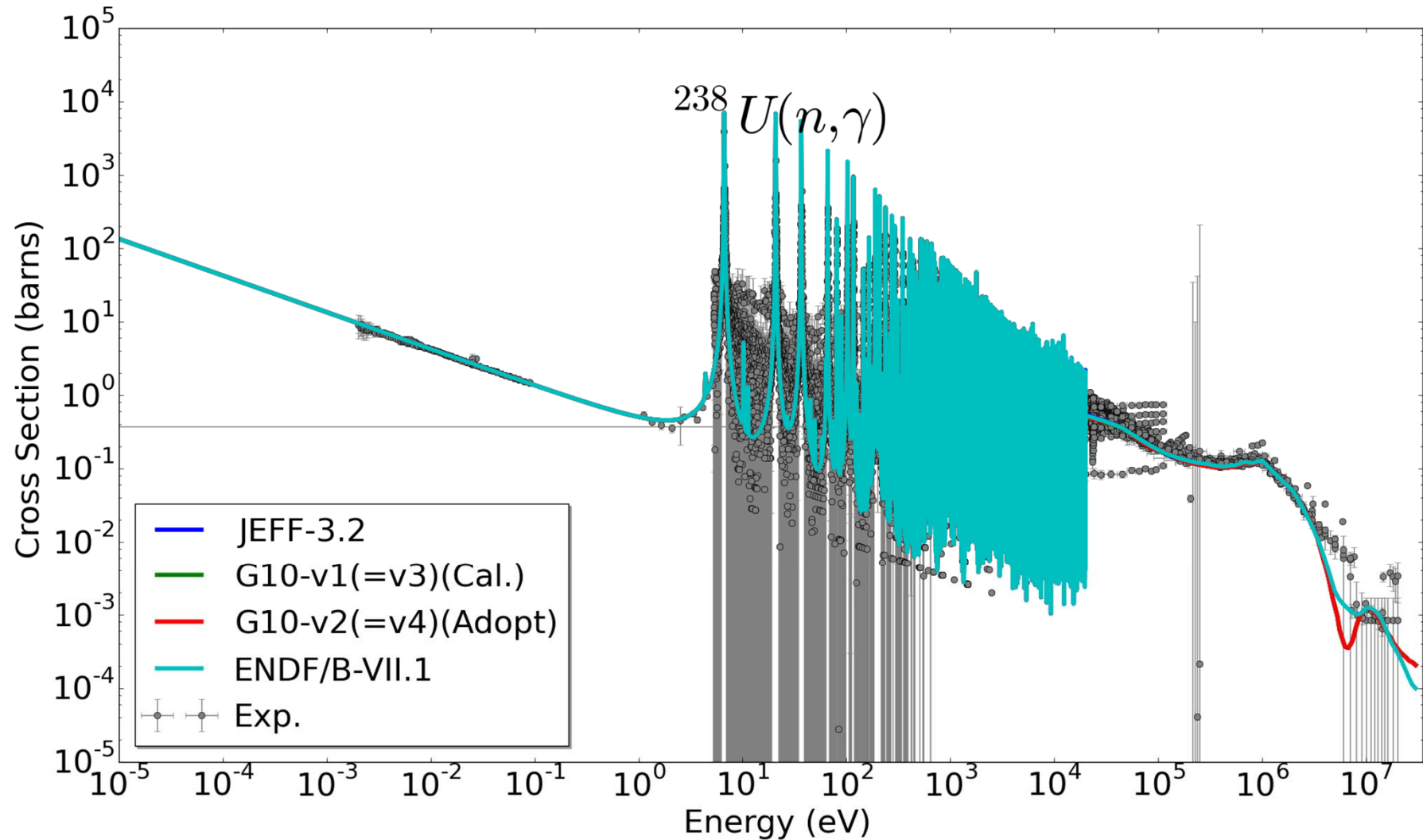
- ◆ Four separate U-238 evaluations
 - ☞ depending on treatment of capture and inelastic scattering cross sections in resonance energy region
- ◆ Two files named G10 and G20
 - ☞ energy boundaries between RR and URR regions of 10 keV and 20 keV

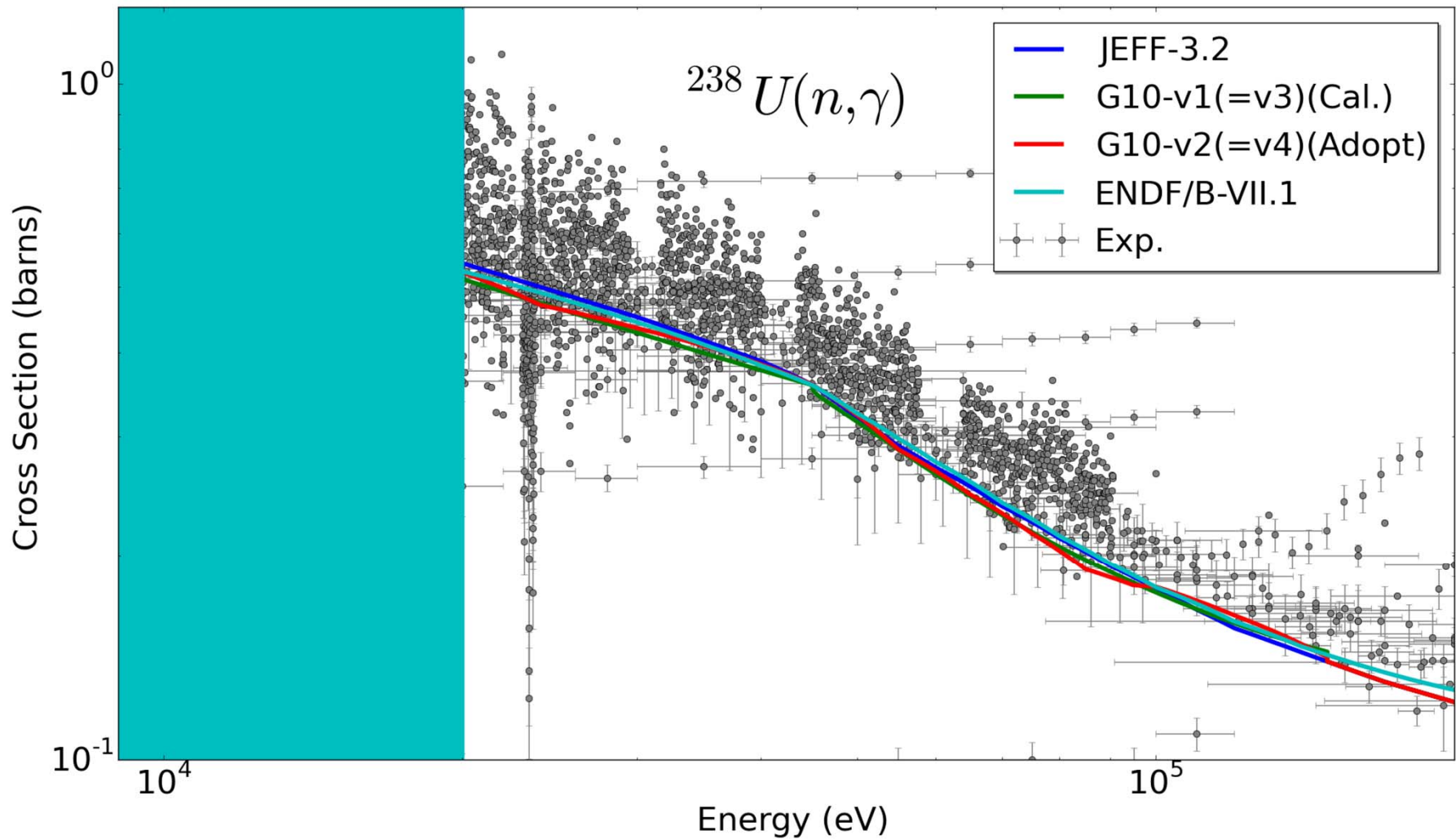
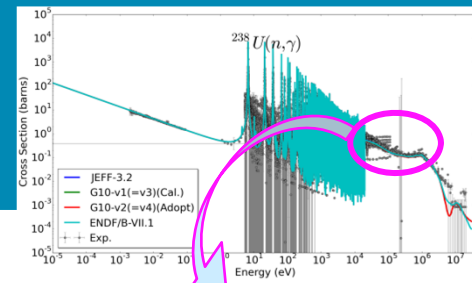


< Summary on G-versions >

Version	Cross Section Evaluation	
	Capture	Inelastic Scattering
G10-1 & G20-1	Calculated (statistical evaluation)	Calculated (statistical evaluation, direct reaction component determined by a DCCOM)
G10-2 & G20-2	Adopted	Calculated
G10-3 & G20-3	Calculated	Adopted
G10-4 & G20-4	Adopted (GMA evaluation of Carlson et al.)	Adopted (recent neutron scattering study of Capote et al.)

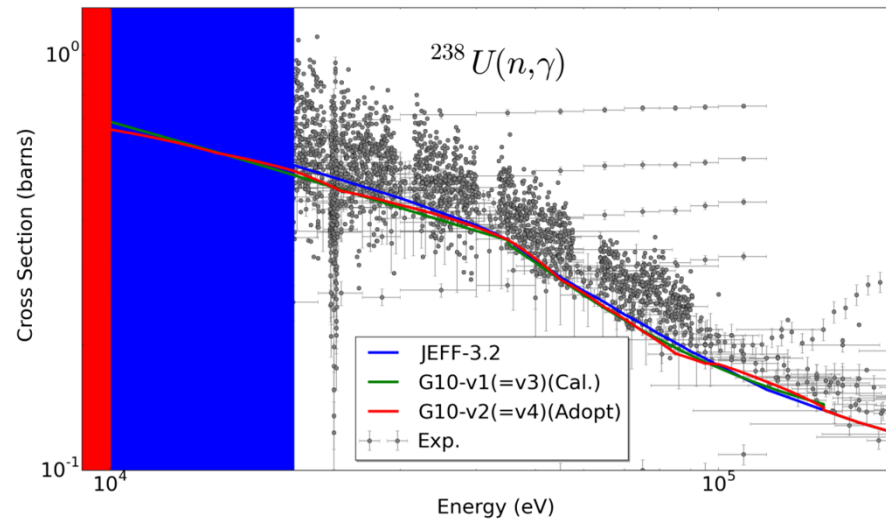
< U-238 Capture Cross Section >



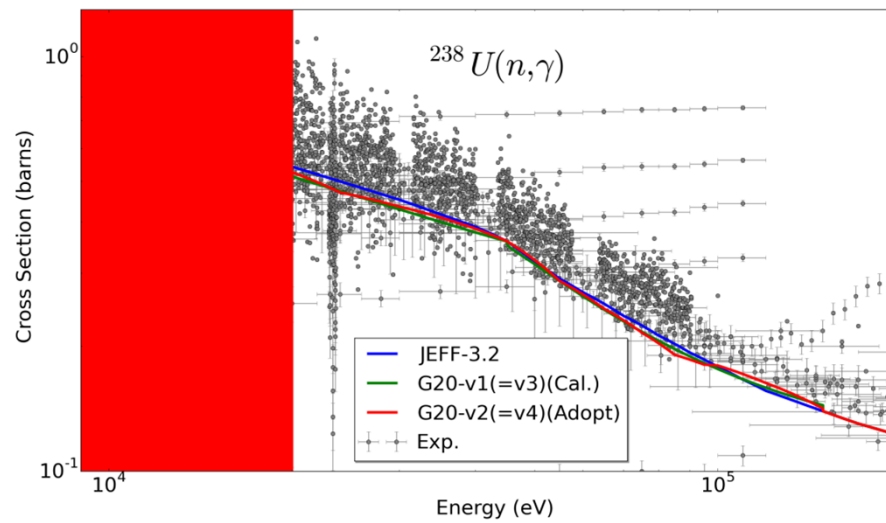




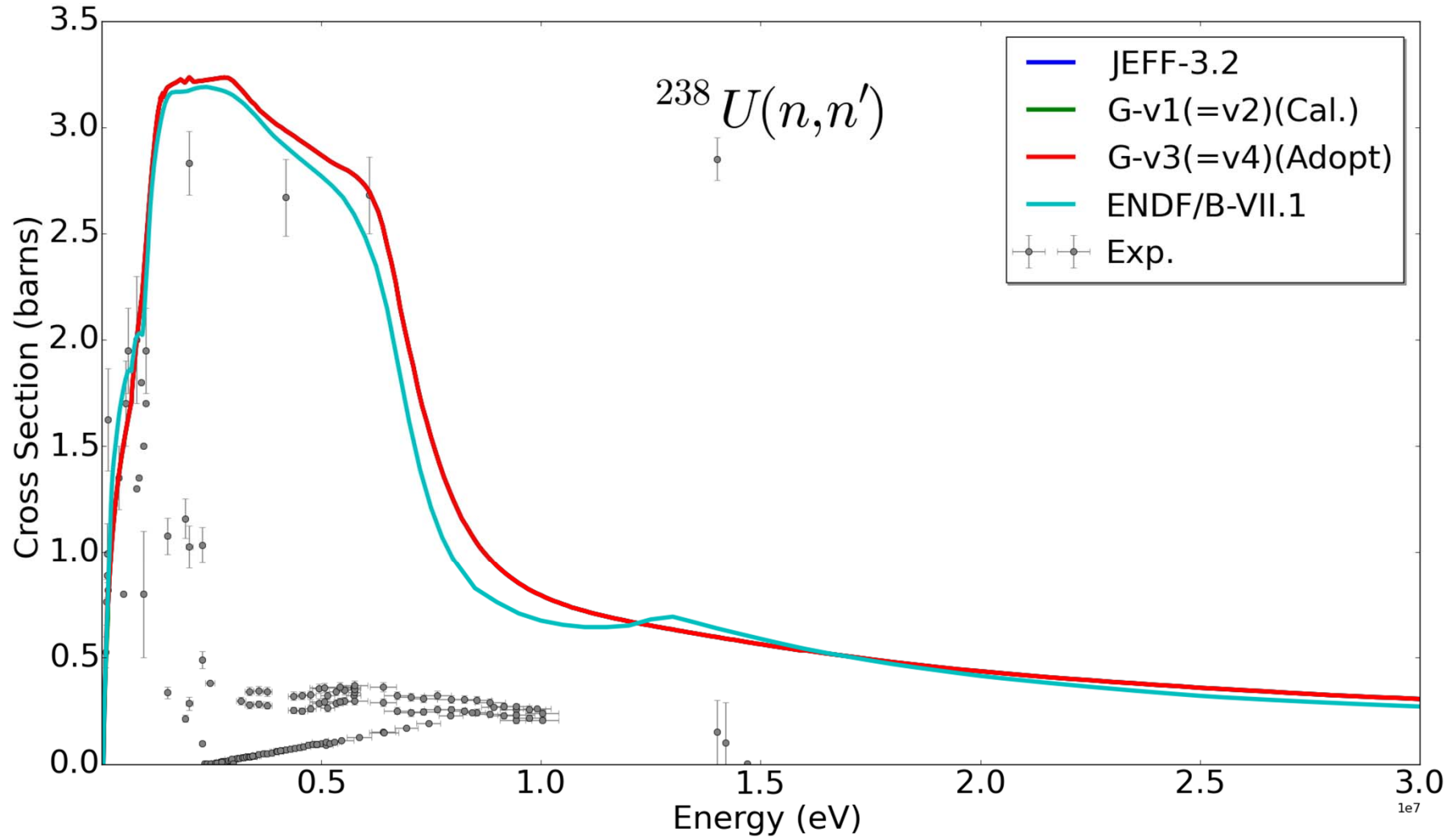
G10

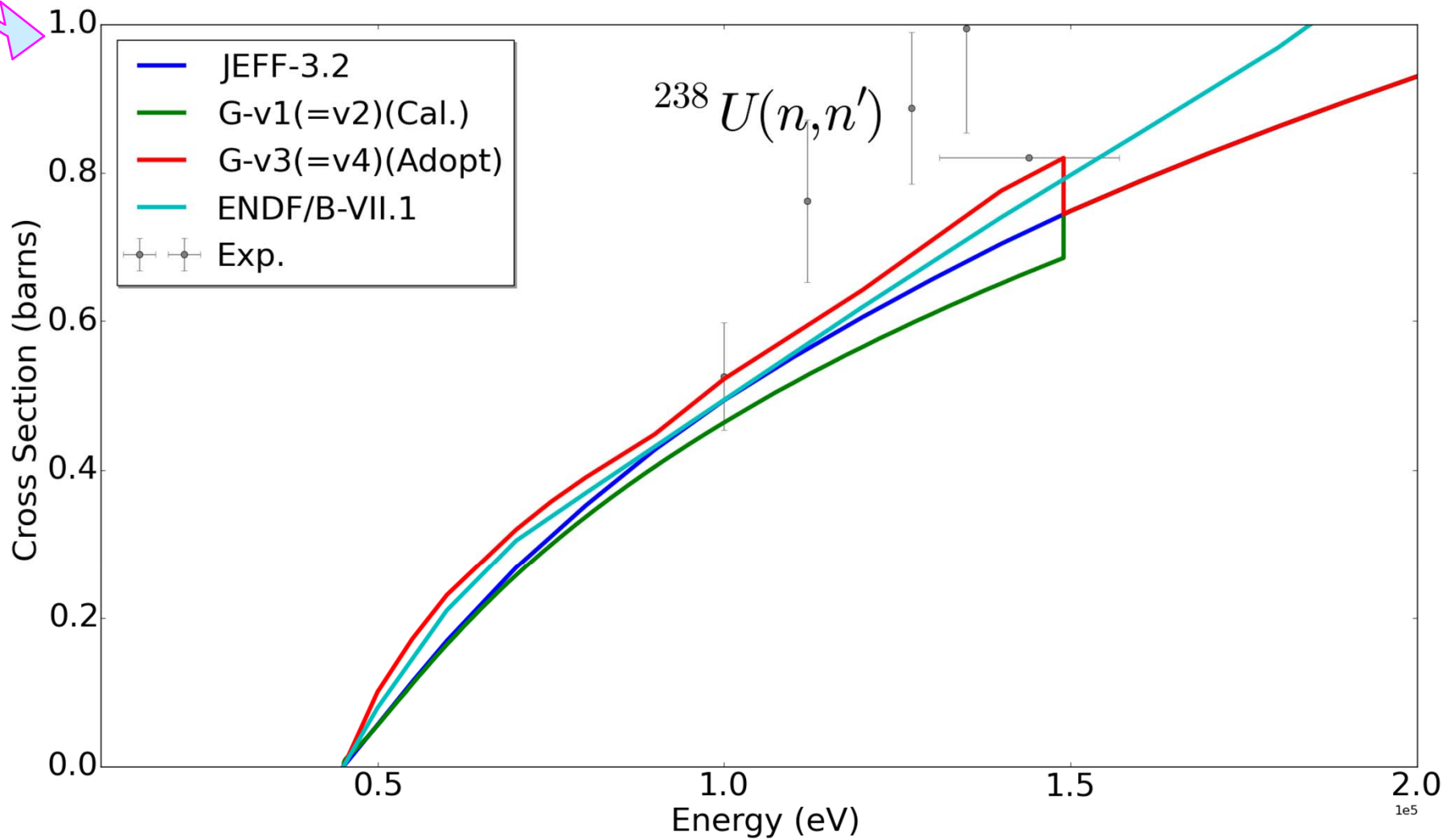


G20



< U-238 Inelastic Scattering Cross Section >





III. Criticality Benchmark Problems

◆ Expanded Criticality Validation Suite

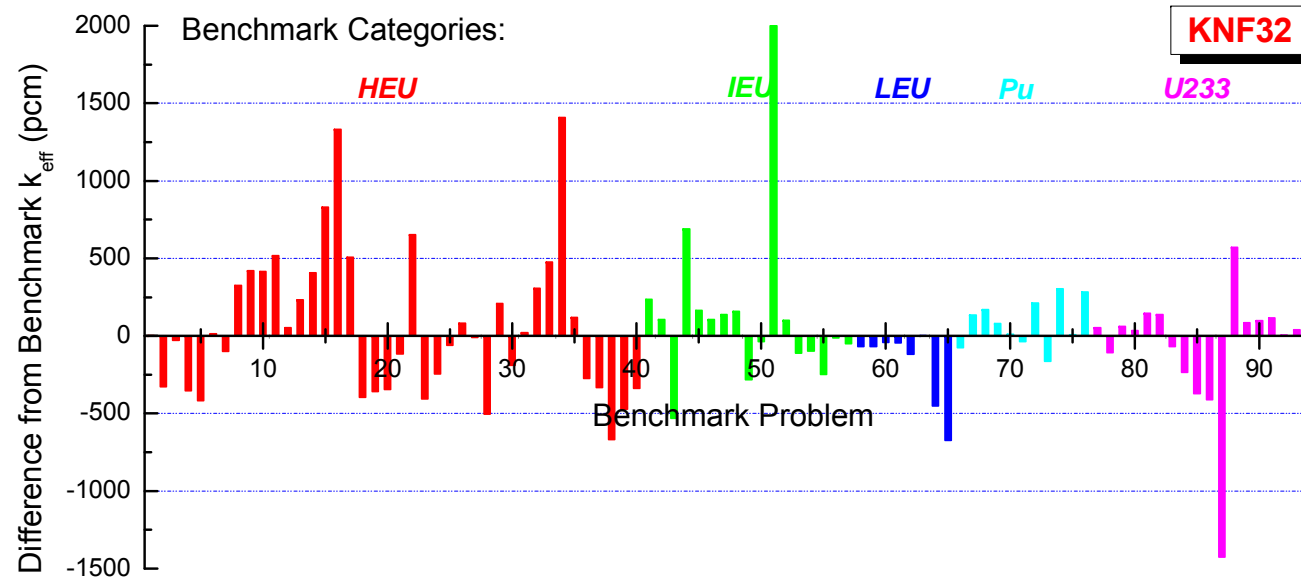
- ☞ to validate MCNP code along with nuclear data libraries
- ☞ 119 criticality benchmark problems taken from ICSBEP
- ☞ Five categories according to principal fuels, i.e., HEU, IEU, LEU, Pu, and U233 systems

◆ Validation Calculations

- ☞ MCNP5
- ☞ Reference Results: JEFF-3.2-based calculation
- ☞ Replace U-238 data with G-versions from reference calculation

Category	Number of Benchmark Problems	
	Validation of U-238	Expanded Suite
HEU	40	40
IEU	17	17
LEU	8	8
Pu	11	36
U233	18	18
Whole	94	119

Reference Calculation Results vs. Benchmark k_{eff}



IV. Validation Results

◆ Overall Performance Tests

☞ Comparison of Root Mean Square (RMS) Errors

☞ Comparison of χ^2 Values

☞ Number of Problems within Certain Confidence Intervals

- Compare $\Delta k = |k_{C,i} - k_{E,i}|$ Vs. *Uncertainty* ($\sigma = \sigma_{exp} + \sigma_{calc}$)
- Within which confidence intervals?

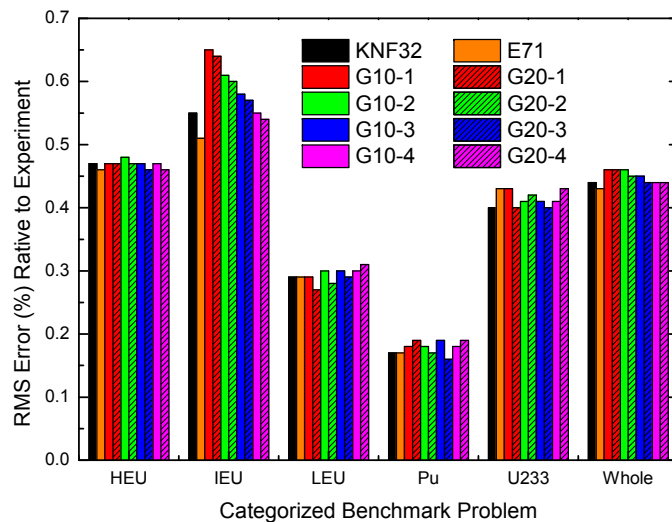
$$\Delta k < 1\sigma \quad \text{or} \quad 1\sigma < \Delta k < 2\sigma \quad \text{or} \quad 2\sigma < \Delta k < 3\sigma \quad \text{or} \quad 3\sigma < \Delta k$$

☞ Ratio of Calculated k_{eff} to Experimental k_{eff}

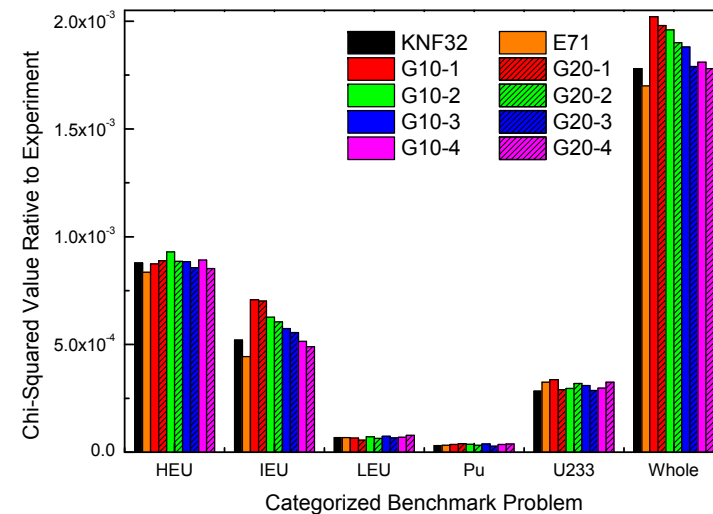
- $Z_i = k_{C,i}/k_{E,i}$
- Average Value
- Standard Deviation

Comparisons of RMS Error & χ^2 Values

RMS Errors



χ^2 Values



$$RMS(\%) = \sqrt{\frac{\sum_{i=1}^N (k_{C,i} - k_{E,i})^2}{N}}$$

$$\chi^2 = \sum_{i=1}^N \frac{(k_{C,i} - k_{E,i})^2}{k_{E,i}}$$

- ✓ G-versions 3 & 4 are more comparable to the reference.
- ✓ Obvious changes by different G-versions of U-238 are shown in IEU systems.
- ✓ Improvements in χ^2 values for whole problems are achieved in G20-3, G10-4, and G20-4.

Number of Problems within Certain Confidence Intervals

Energy Boundary of 10 keV between RR & URR

Confidence Interval	F32	E71	G10-1	G10-2	G10-3	G10-4
< 1 σ	57	58	54	56	56	53
1 σ ~ 2 σ	23	23	27	26	27	28
2 σ ~ 3 σ	11	10	10	9	8	10
> 3 σ	3	3	3	3	3	3

Energy Boundary of 20 keV between RR & URR

Confidence Interval	F32	E71	G20-1	G20-2	G20-3	G20-4
< 1 σ	57	58	52	59	56	60
1 σ ~ 2 σ	23	23	30	23	27	23
2 σ ~ 3 σ	11	10	8	9	8	7
> 3 σ	3	3	4	3	3	4

- ✓ U-238 evaluations with energy boundary of 20 keV tend to produce more reliable MCNP calculation results below 2 STD than 10 keV.
- ✓ Enhancements were seen in G10-3, G20-3, and G20-4 in comparison to JEFF-3.2.

Z₁, Ratio of Calculated k_{eff} to Experimental k_{eff}

Average

Category	F32	G-version 1		G-version 2		G-version 3		G-version 4	
		10keV	20keV	10keV	20keV	10keV	20keV	10keV	20keV
HEU	1.0006	1.0006	1.0007	1.0006	1.0006	1.0006	1.0006	1.0005	1.0005
IEU	1.0014	1.0018	1.0019	1.0015	1.0017	1.0017	1.0016	1.0014	1.0013
LEU	0.9982	0.9985	0.9985	0.9982	0.9984	0.9981	0.9984	0.9984	0.9984
Pu	1.0008	1.0009	1.0010	1.0008	1.0007	1.0009	1.0006	1.0008	1.0009
U233	0.9994	0.9991	0.9991	0.9992	0.9991	0.9991	0.9990	0.9992	0.9991
Whole	1.0003	1.0004	1.0005	1.0003	1.0004	1.0004	1.0003	1.0003	1.0003

STD

Category	F32	G-version 1		G-version 2		G-version 3		G-version 4	
		10keV	20keV	10keV	20keV	10keV	20keV	10keV	20keV
HEU	0.0046	0.0046	0.0047	0.0048	0.0047	0.0047	0.0046	0.0047	0.0046
IEU	0.0053	0.0062	0.0061	0.0059	0.0057	0.0055	0.0055	0.0053	0.0052
LEU	0.0023	0.0024	0.0022	0.0024	0.0024	0.0024	0.0024	0.0024	0.0027
Pu	0.0014	0.0016	0.0016	0.0016	0.0016	0.0016	0.0015	0.0016	0.0016
U233	0.0039	0.0042	0.0039	0.0040	0.0041	0.0040	0.0039	0.0040	0.0042
Whole	0.0043	0.0046	0.0046	0.0046	0.0045	0.0045	0.0044	0.0044	0.0043



- ◆ Influence due to Extension of Energy Boundary between RR and URR from 10 to 20 keV
 - ☞ Important Factor to be Settled on after Validation of New U-238 Evaluations
 - ☞ Compare relative improvements (%) in
 - RMS Errors
 - χ^2 Values

Extension of Energy Boundary between RR and URR

Category	Relative Improvements (%) in RMS Errors			
	G-version 1	G-version 2	G-version 3	G-version 4
HEU	0.00	2.08	2.13	2.13
IEU	1.54	1.64	1.72	1.82
LEU	6.90	6.67	3.33	-3.33
Pu	-5.56	5.56	15.79	-5.56
U233	6.98	-2.44	2.44	-4.88
Whole	0.00	2.17	2.22	0.00

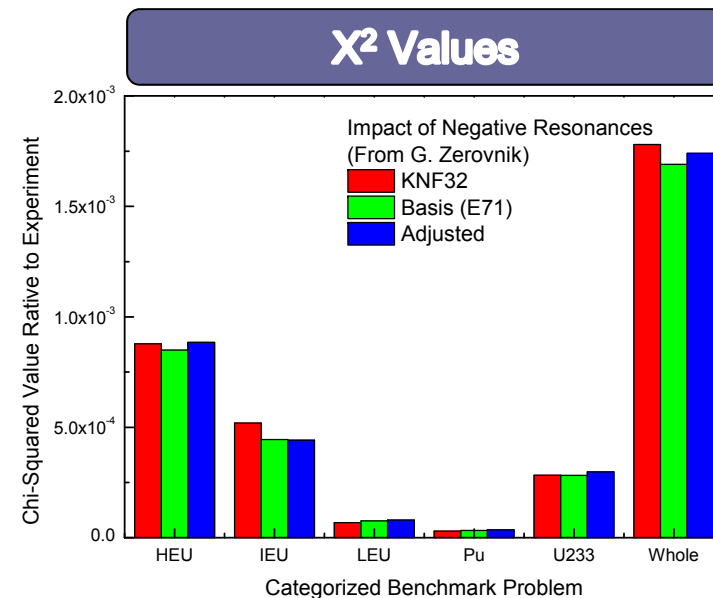
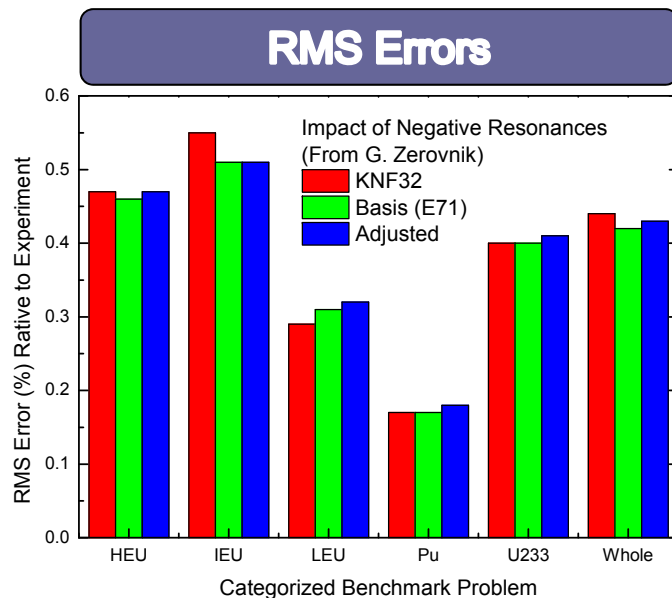
Category	Relative Improvements (%) in χ^2 Values			
	G-version 1	G-version 2	G-version 3	G-version 4
HEU	-1.83	4.74	3.17	4.38
IEU	0.85	3.35	3.31	4.85
LEU	14.18	9.99	10.20	-12.52
Pu	-10.89	13.94	28.46	-7.10
U233	13.69	-7.43	7.12	-9.43
Whole	1.98	3.06	4.79	1.66

- ✓ Adoption of 20 keV could be more efficient for all G-versions than 10keV.
- ✓ Better improvements were found in G-versions 2 & 3.
- ✓ Especially for G-version 3, positive improvements were achieved in every benchmark categories.

◆ Impact of Negative Resonances

☞ Test evaluation based on ENDF/B-VII.1 by G. Zerovnik

- some adjustments to negative resonances to match the Olsen transmission data while maintaining thermal data (capture and coherent scattering length)
- Two files (basis & adjusted) only differ in the parameters of the bound states.





Number of Problems within Certain Confidence Intervals

Confidence Interval	KNF32	Basis(E71)	Adjusted
< 1 σ	57	56	58
1 σ ~ 2 σ	23	24	22
2 σ ~ 3 σ	11	11	9
> 3 σ	3	3	5

Z_i, Ratio of Calculated k_{eff} to Experimental k_{eff}

Category	Average			Standard Deviation		
	KNF32	Basis(E71)	Adjusted	KNF32	Basis(E71)	Adjusted
HEU	1.0006	1.0002	1.0002	0.0046	0.0046	0.0047
IEU	1.0014	1.0016	1.0017	0.0053	0.0048	0.0048
LEU	0.9982	0.9982	0.9980	0.0023	0.0025	0.0025
Pu	1.0008	1.0001	0.9999	0.0014	0.0017	0.0018
U233	0.9994	0.9989	0.9991	0.0039	0.0038	0.0040
Whole	1.0003	1.0000	1.0000	0.0043	0.0042	0.0043

V. Conclusions



- ◆ G-versions 3 & 4 showed better performances than the others by comparing RMS errors, χ^2 values, and number of problems within certain confidence intervals.
 - ☞ Adoption of inelastic evaluation from recent neutron scattering study of Capote et al. might be quite pertinent to new U-238 evaluations.
- ◆ Extension of energy boundary between RR and URR from 10 to 20 keV was efficient for all G-versions of U-238.
- ◆ **G20-3** & **G20-4** would be the best options among all G-versions from our validation study.
- ◆ Further studies are required to see how G-versions would be working in some specific benchmark cases strongly affected by URR cross sections.