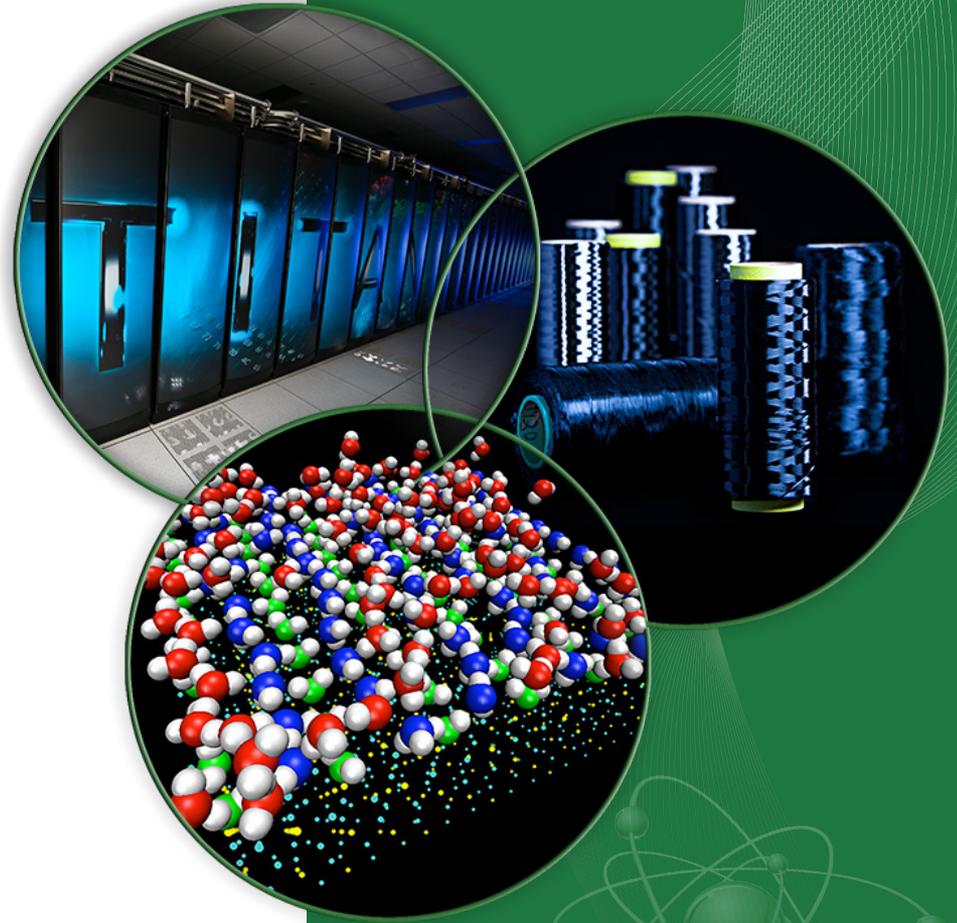


Cross Section Evaluation of ^{40}Ca for Neutron Energies up to 1.5 MeV and Validation of Tungsten Cross Sections up to 100 keV

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Sandia National Laboratories
Albuquerque, March 2016

Outline

- Motivation
- Nuclear data evaluation overview for ^{40}Ca
- Evaluation procedure with SAMMY
 - Channels definition
 - Experimental data overview
- Cross section evaluation work on ^{40}Ca (results)
- Validation work on $^{182-184,186}\text{W}$ cross sections (results)
- Conclusions

Motivation

- **Calcium**

- present in structural materials such as concrete and admixed material in waste streams
- neutron-absorbing element that can influence the reactivity of systems with fissionable material
- need for improved cross sections is identified specifically for *Hanford Plutonium Finishing plant* and *Hanford Tank Farms* in the DOE complex
- Need for evaluated covariance data to support sensitivity/uncertainty (S/U) analyses

- **Tungsten**

- structural material present in process facilities and also of essential importance for shielding
- long-standing computational bias associated with tungsten in benchmark calculations (poor performance of capture data)
- Need for evaluated covariance data for S/U analyses

^{40}Ca Cross Section Evaluation Overview

(in ENDF/B-VII.1 library)

- Current status of ^{40}Ca evaluation in ENDF/B-VII.1 library (2011)
 - Evaluation work taken from JEFF-3.1 (May 2005, A.J. Koning)
 - Original data taken from JEFF-3.1 (Oct. 2004)
 - Resonance parameters (MF2/MT151) : JENDL-3.3 (2002) for $E < 500$ keV
 - Total cross section (MF3/MT1) : ENDF/B-VI.8 (2001) for $E < 20$ MeV
 - All other data : produced by TALYS code (May 2005)
- In ENDF/B-VII.1 library resonance parameters for Multi Level Breit Wigner formula taken from the recommended data (Mughabghab, 1981)
- No covariance data given in the ENDF/B-VII.1 library

⁴⁰Ca Cross Section Evaluation Overview

(reaction channels)

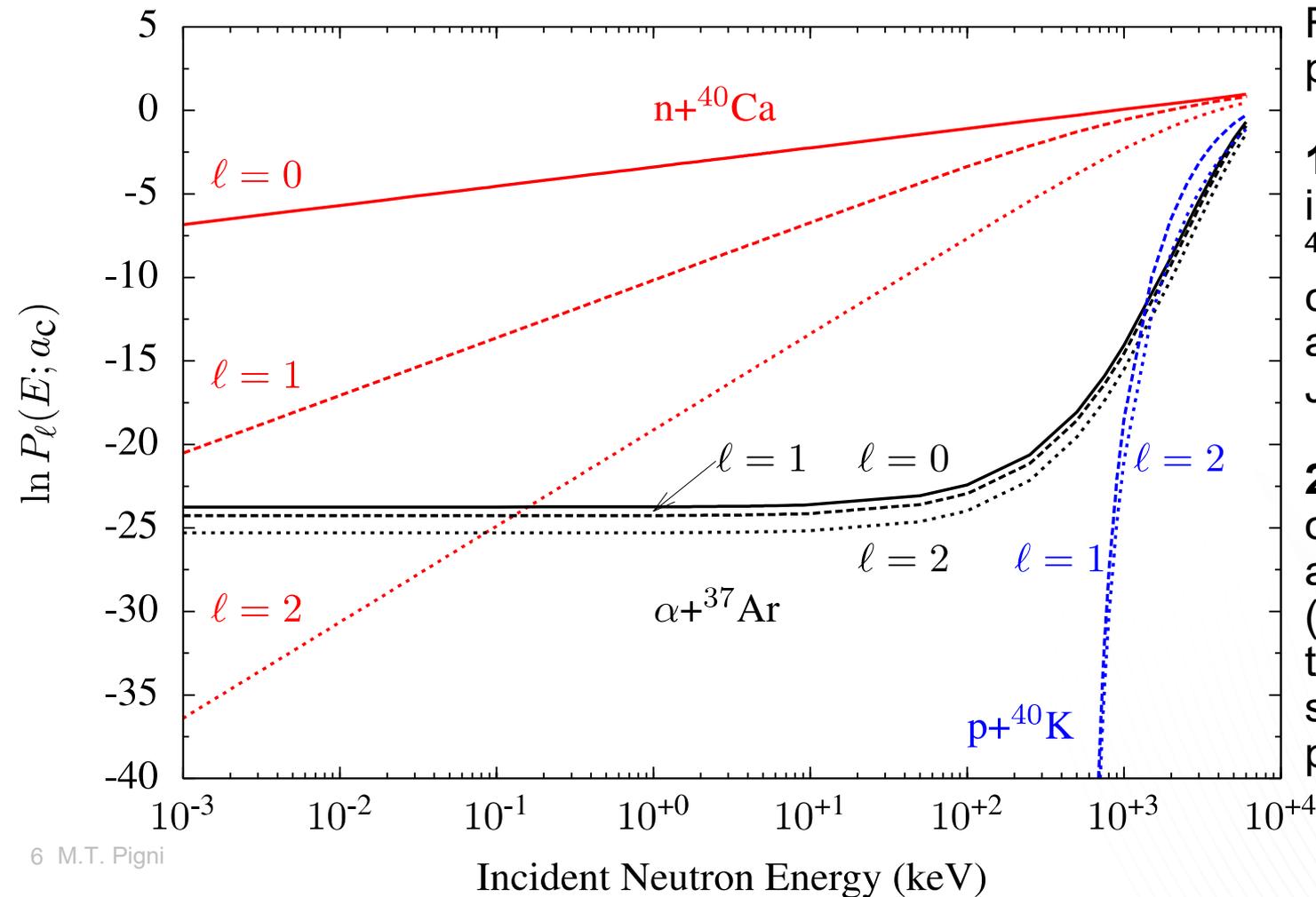
Reaction product	Q-value (keV)	Threshold (keV)
⁴¹ Ca+ γ	+8362.82	0.0
³⁷ Ar+ α_0	+1747.66	0.0
⁴⁰ K+p ₀	-528.55	541.89
⁴⁰ Ca+n ₁	-3352.62	3437.17
³⁹ Ca+2n	-15635.0	16029.74

- Besides the elastic channel, three reactions (in red) are energetically possible in the neutron energy region up 1.5 MeV
 - α -particle emissions (Q-value>0) also at sub-thermal and thermal energies
- For charged particle reaction channels penetrability factors defined by the Coulomb functions F_1 and G_1 :

$$P_1 = \rho / (F_1 + G_1)$$

$n+^{40}\text{Ca}$ Channel Definitions (particle pairs)

- The magnitude of the penetrability factors determines the strength of the partial-wave components of the quasi-stationary compound state.



For $p+^{40}\text{K}$ particle-pair

1) s-wave are not included because ^{40}K has spin $I^\pi=4^-$ coupling to have total angular momentum $J^\pi=7/2^-$ and $9/2^-$

2) careful treatment of the partial widths at threshold energies (about 0.5 MeV) due to the considerable small values of the penetrability factors

$n+^{40}\text{Ca}$ Resonance Evaluation

- Transmission and capture cross section measurements performed at Geel for $^{\text{nat}}\text{Ca}$ in the energy range up to 1 MeV (Guber)
 - Measurements of Calcium using metallic samples
 - The samples are in Al canning due to reactivity with air
 - Transmission experiments w/ different sample thickness (flight path 50 m)
 - Neutron capture using detector system (flight path 60 m)

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- Early high-resolution total cross section measurements by
 - Cierjacks (1968, KIT): $^{\text{nat}}\text{Ca}(n,\text{tot})$
 - Perey (1972, ORELA): $^{\text{nat}}\text{Ca}(n,\text{tot})$
 - Singh (1975): $^{\text{nat}}\text{Ca}(n,\text{tot})$
 - Johnson (1978, ORELA): $^{40}\text{Ca}(n,\text{tot})$

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- Used formalism of Reich-Moore approximation
- Included (n,α) and (n,p) channels

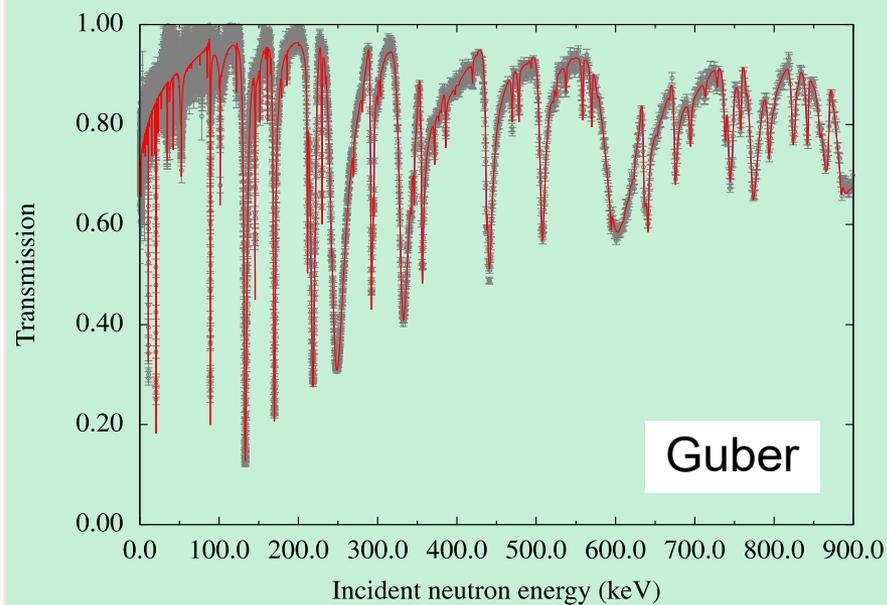
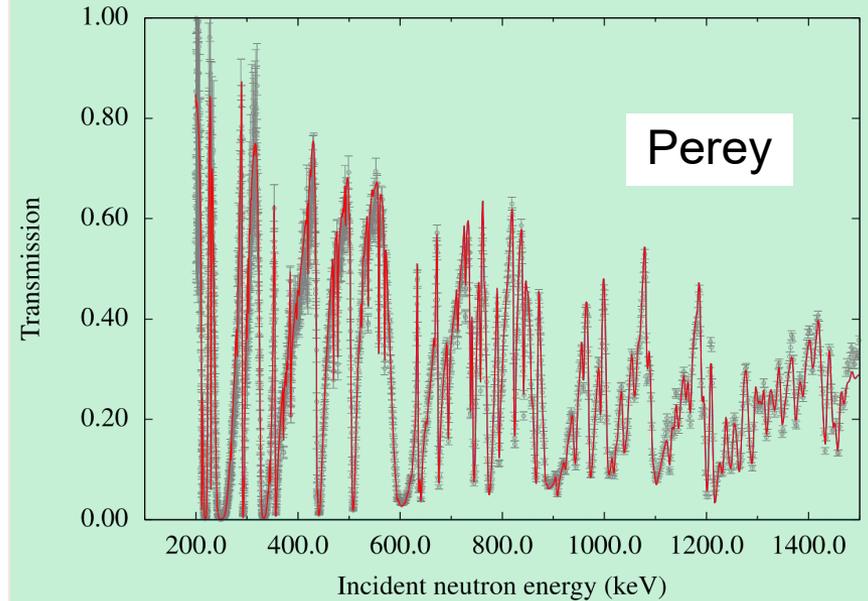
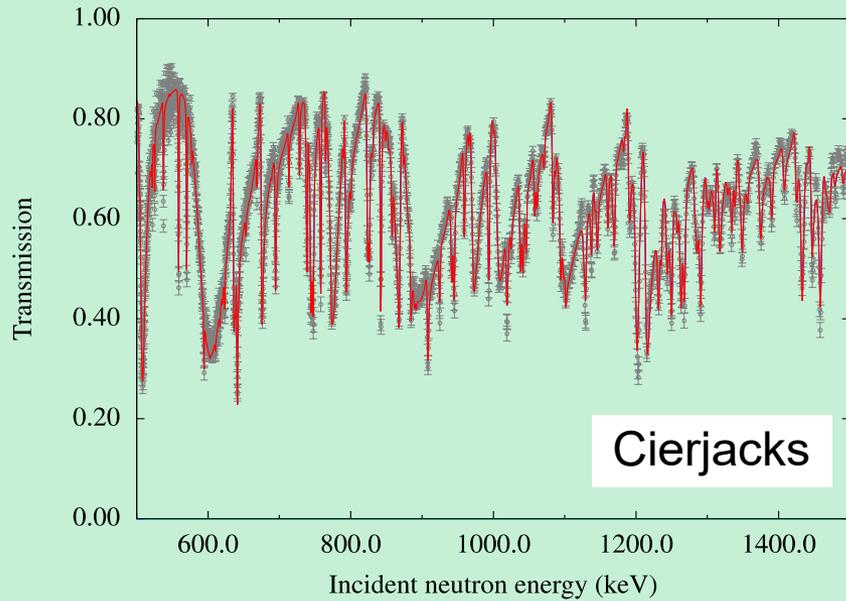
n+⁴⁰Ca Experimental Data Overview

Sample	Author (Fac./Year)	Exp. range (keV) E _{fit}	Reaction Thick.(at/b)	No. data (No. data E _{fit})	X ^{2**} (ave. unc.)	Norm.
natCa*	Cierjacks (KIT/1968)	500-31000 (1500)	Total 0.21326	5113 (2476)	5.39 (1.5%)	0.96
natCa*	Perey (ORNL/1972)	200-29000 (1500)	Total 0.7028	3501 (2420)	2.07 (16.4%)	0.97
⁴⁰ Ca*	Johnson (ORNL/1973)	40-6000 (1500)	Total 0.0656	7709 (6502)	6.12 (3.8%)	0.98
natCa*	Singh (NSC/1974)	1.6-550 (550)	Total 0.029762	674 (674)	4.15 (10.0%)	0.99
natCa	Guber (GEEL/2014)	0.02-1000 (900)	Trans 0.11644	28764 (28672)	1.08 (2.6%)	0.97
natCa	Guber (GEEL/2014)	0.02-600 (350)	Capture 0.01674	20776 (19930)	1.42 (14.8%)	1.00
natCa	Guber (GEEL/2015)	0.01-600 (350)	Capture 0.10971	17316 (16471)	1.86 (17.2%)	1.00

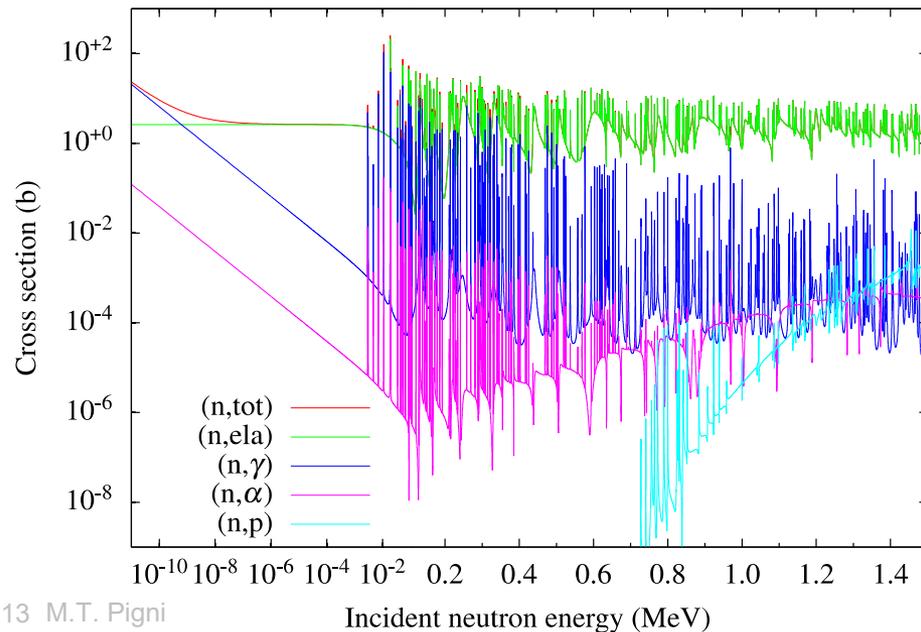
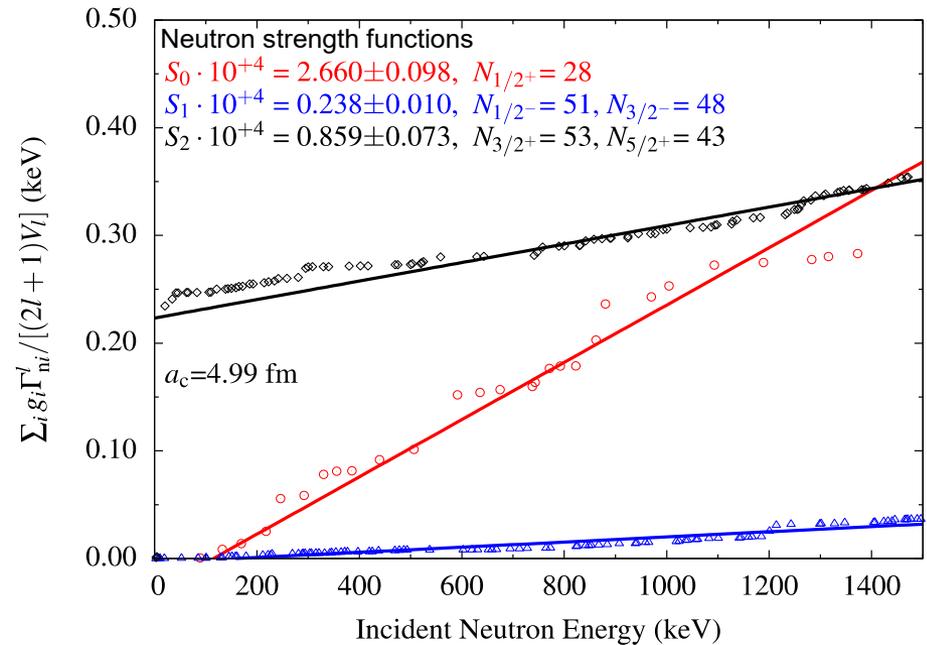
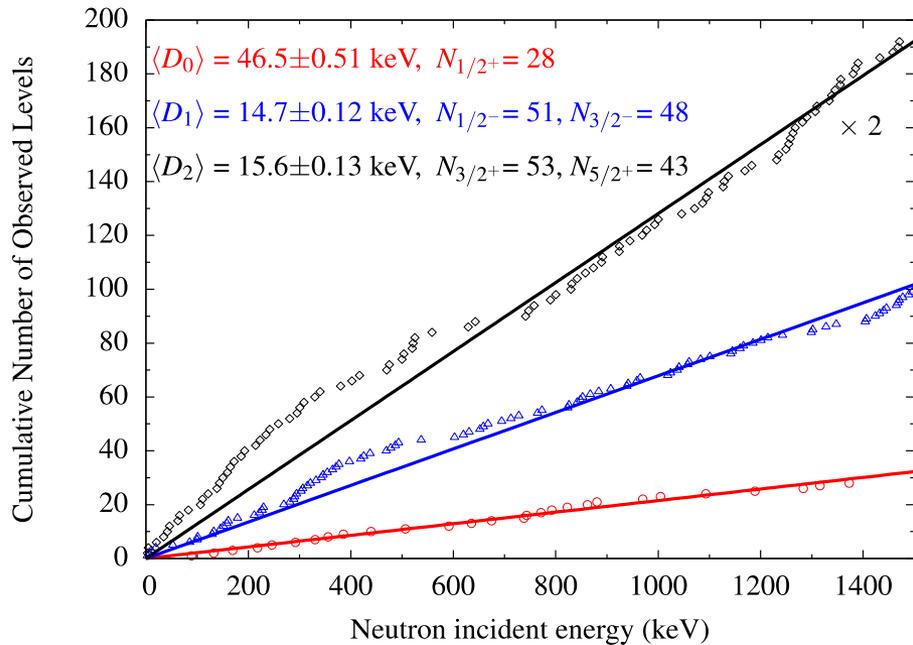
* Retrieved from EXFOR library

** up to 1500 keV

$n+^{40}\text{Ca}$ Cross section evaluation work (results)

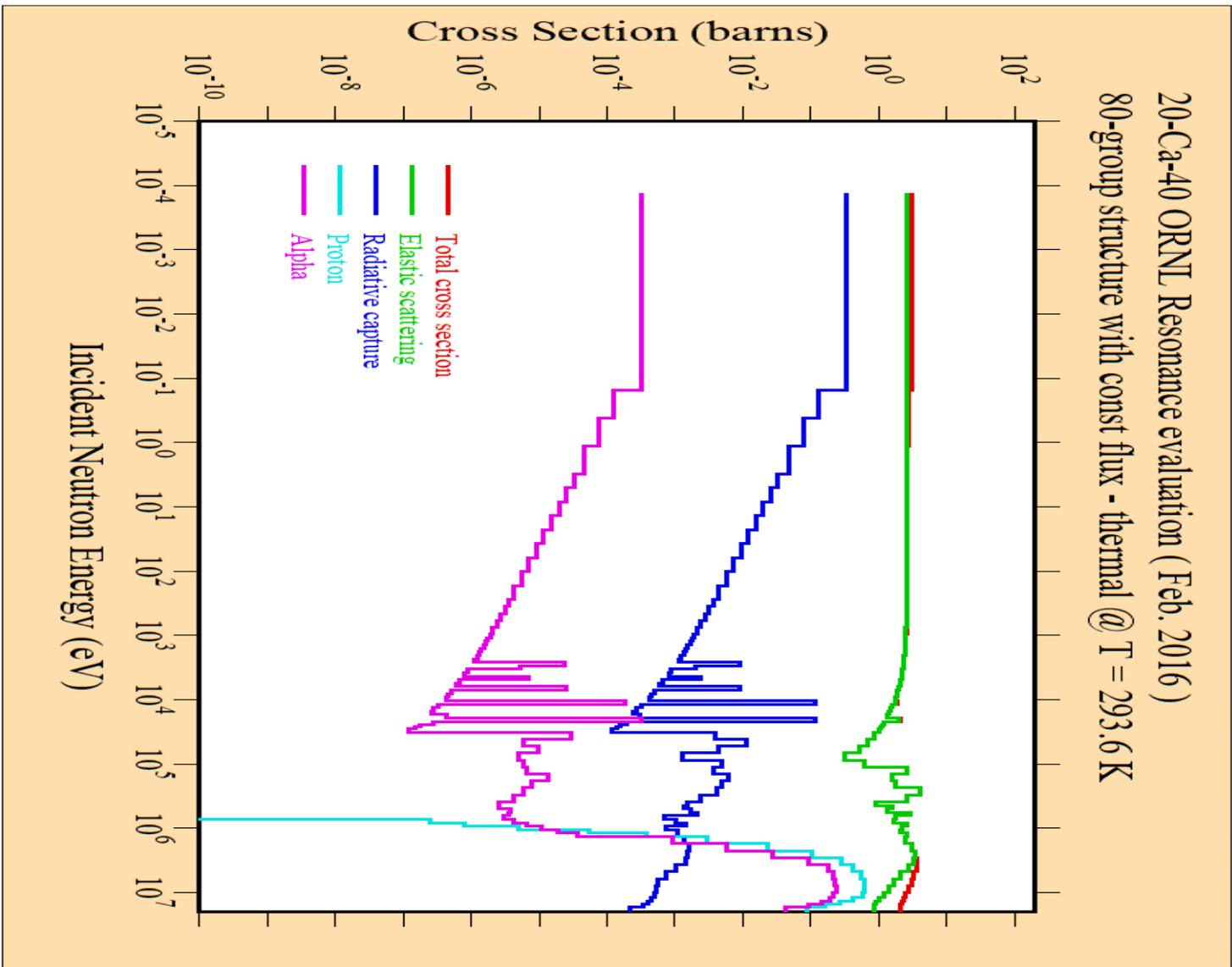


$n+^{40}\text{Ca}$ evaluation statistics

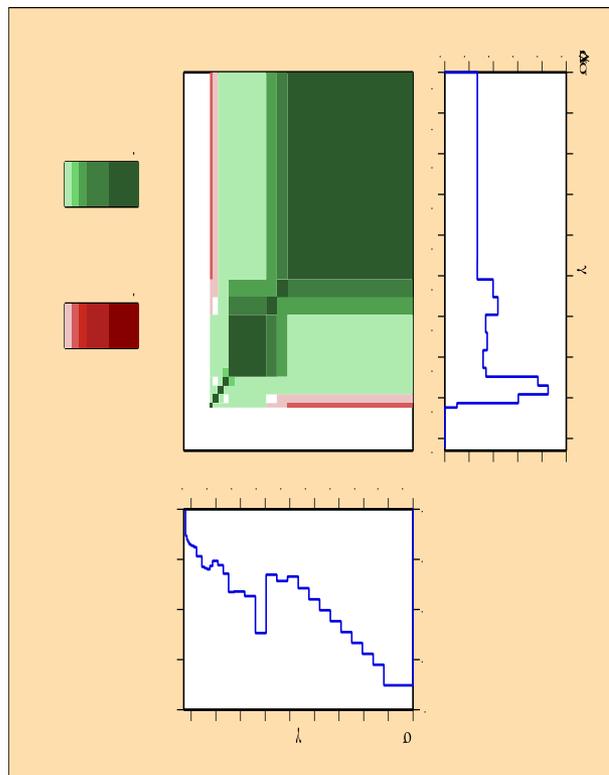


- 7 experimental data sets (5 transmission and 2 capture) included in the cross section evaluation up to 1.5 MeV
- 5 reaction channels (2 for charged-particle emission)
- Total number of levels : 223
- Reich-Moore formalism used
- ENDF format : LRF=7, LCOMP=1

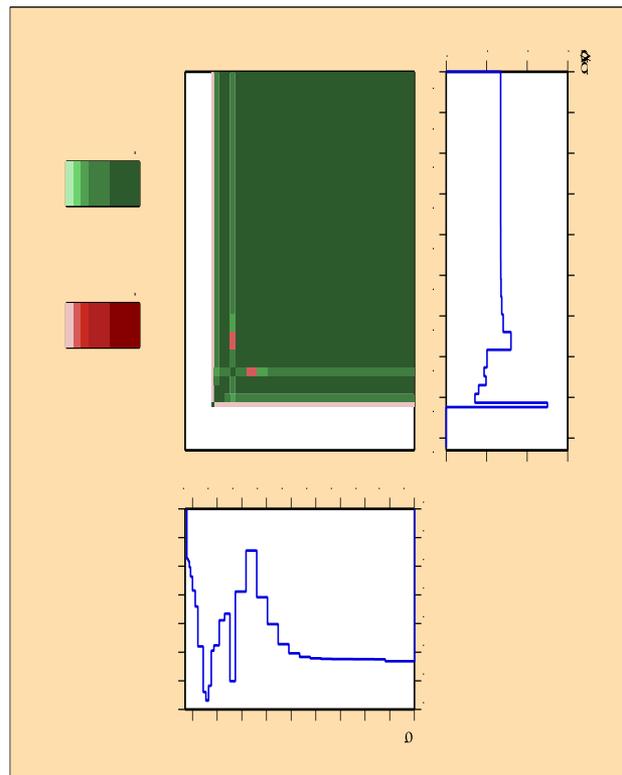
$n+^{40}\text{Ca}$ cross section (up to 20 MeV) and covariances (up 1.5 MeV)



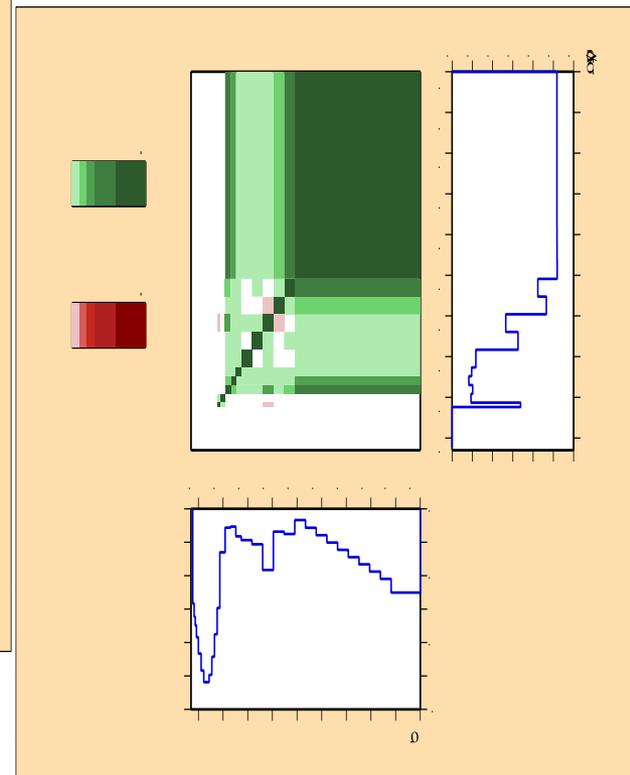
$n+^{40}\text{Ca}$ cross section (up to 20 MeV) and covariances (up 1.5 MeV)



Capture-Capture



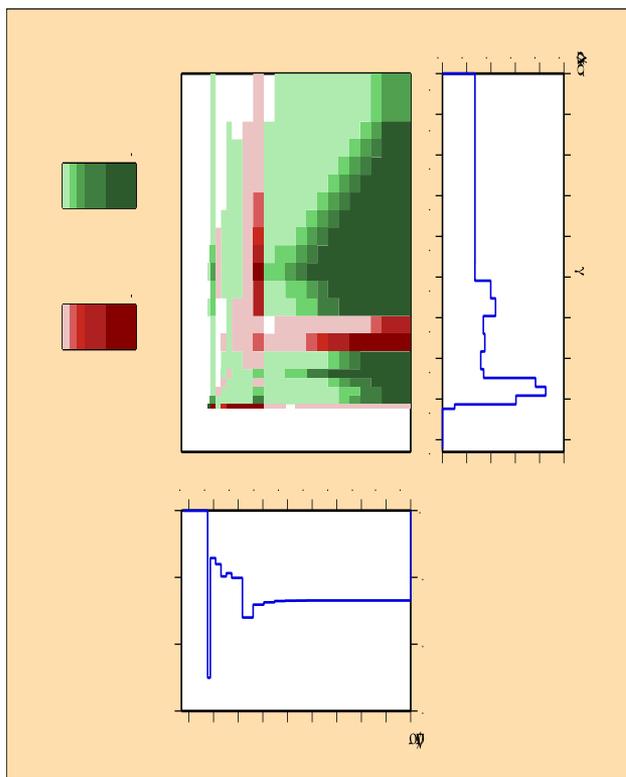
Elastic-Elastic



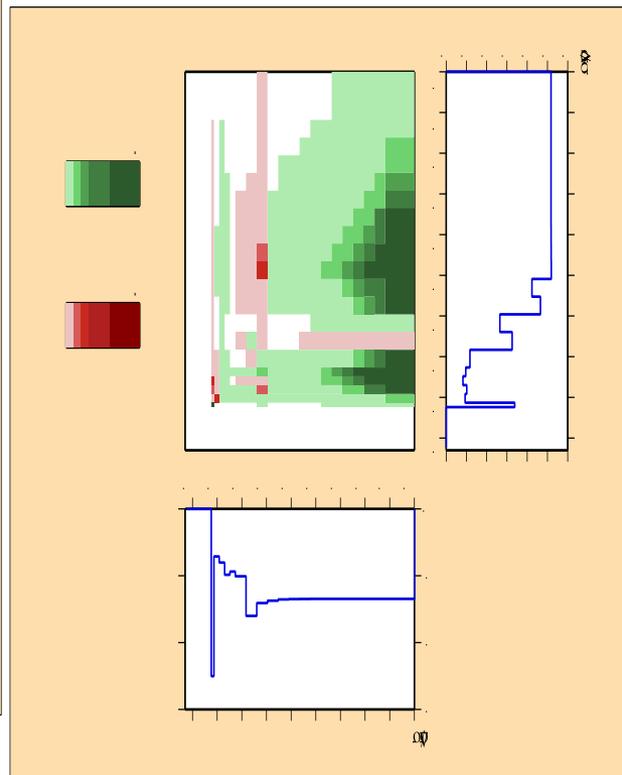
α - α

33-group representation ($T=293.6$ K)

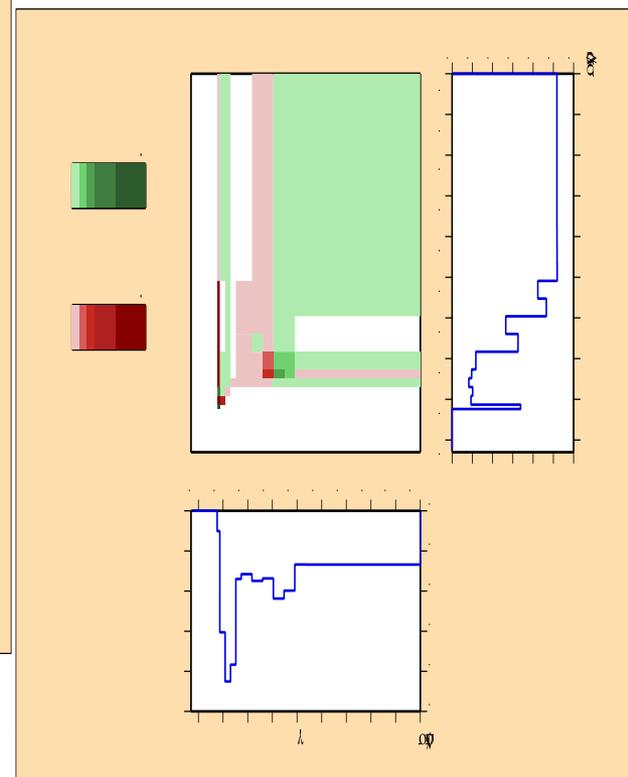
$n+^{40}\text{Ca}$ cross section (up to 20 MeV) and covariances (up 1.5 MeV)



Capture-Elastic



α -Elastic



α -Capture

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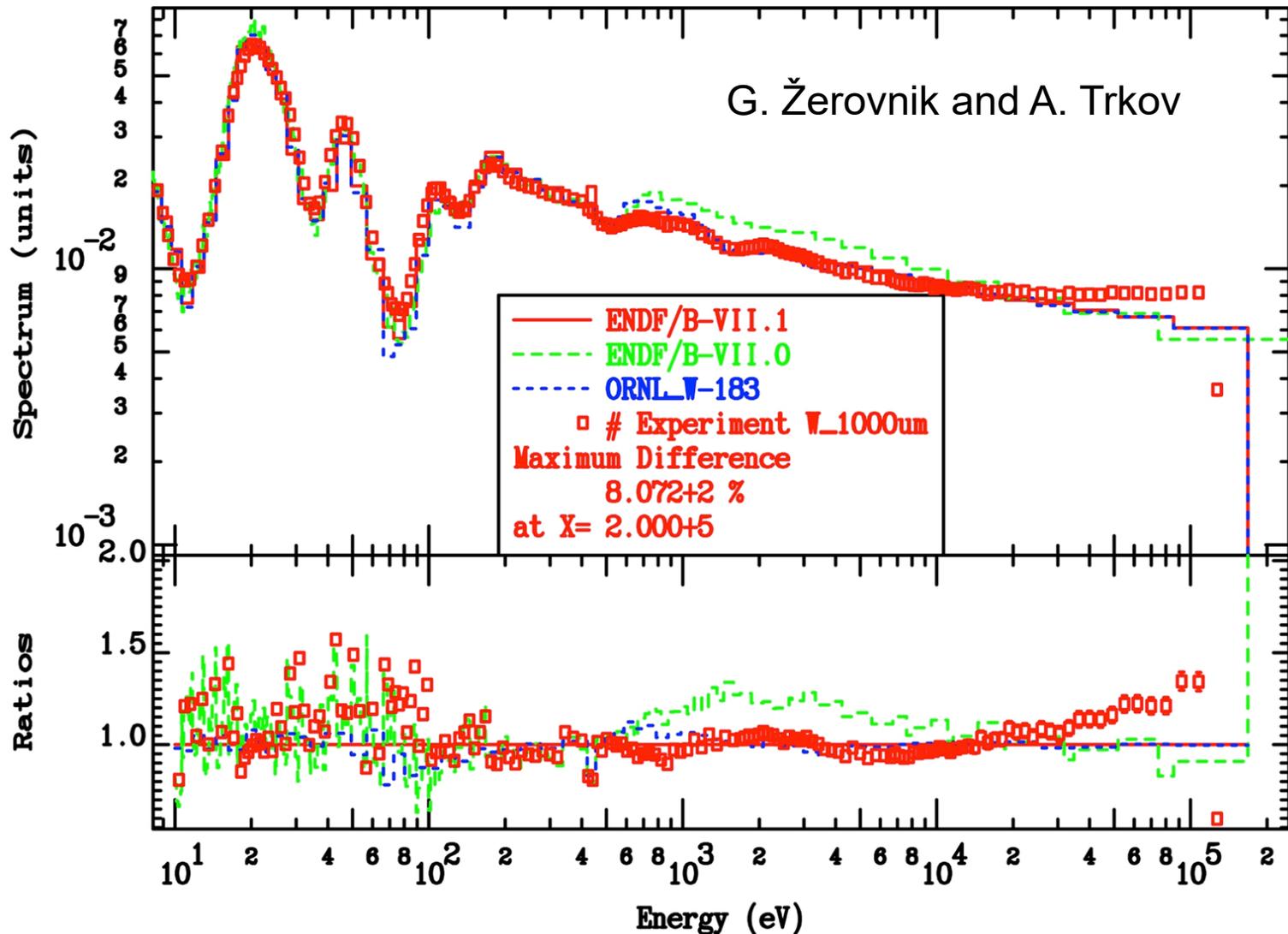
Validation of Tungsten Evaluations

- Four Tungsten evaluations, namely $^{182,183,184,186}\text{W}$, were completed in August 2014
- Three reference published papers
 - M.T. Pigni et al., PHYSOR 2012 - Knoxville, TN April 15-20 2012
 - M.T. Pigni et al., International Conference on Nuclear Data for Science and Technology (ND2013), New York, NY March 4-8 2013
 - M.T. Pigni et al., International Conference on Nuclear Criticality Safety (ICNC2015), Charlotte, NC September 13-17, 2015
- Preliminary validation on ^{183}W in 2013
- Validation on the set of four tungsten evaluations started in November 2015 (thanks to G. Žerovnik, IRMM)
 - Submitted paper to ND2016.

Preliminary validation on ^{183}W (2013)

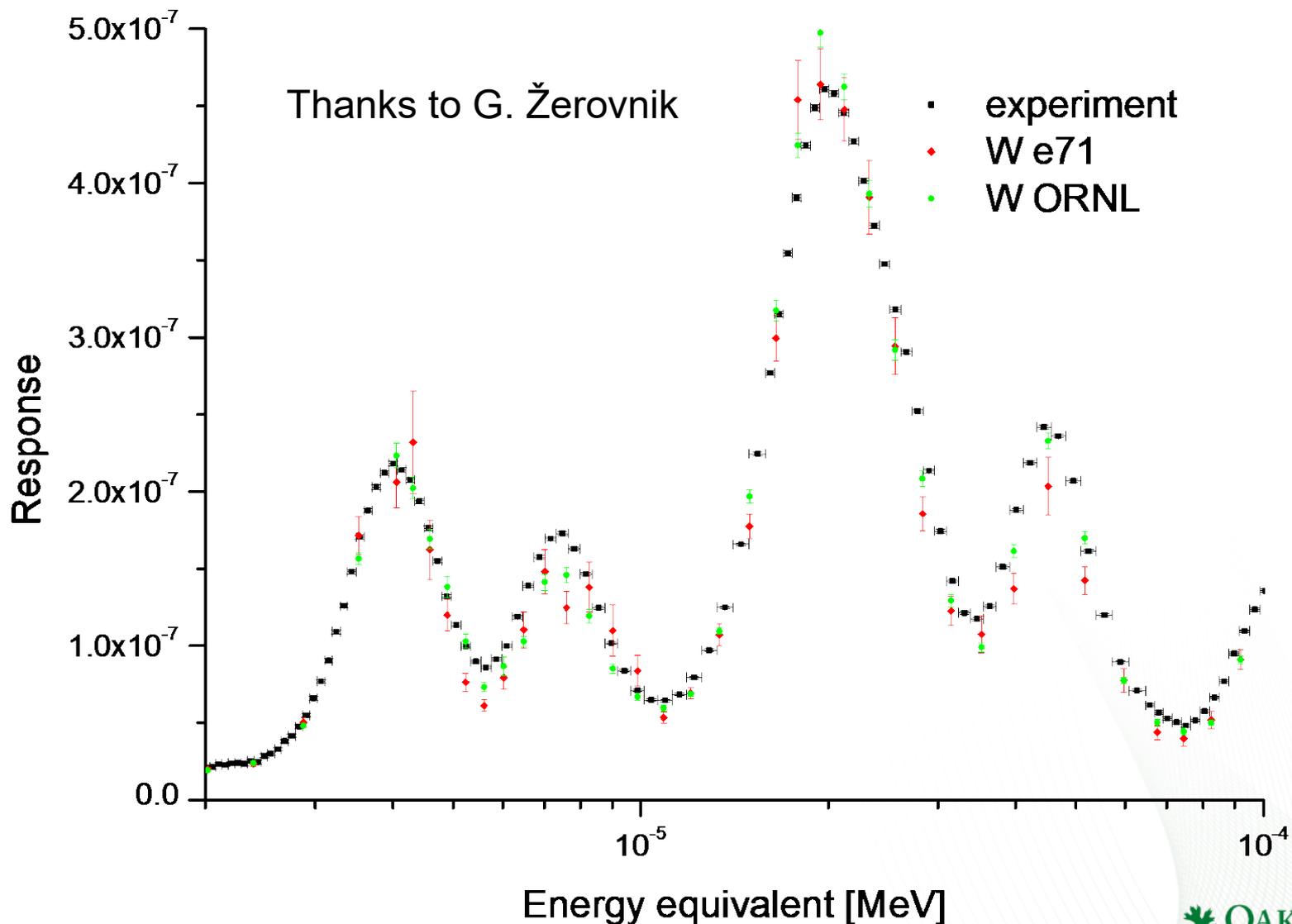
Grenoble Lead Slowing-down Spectrometer
W 1000 um sample

G. Žerovnik and A. Trkov



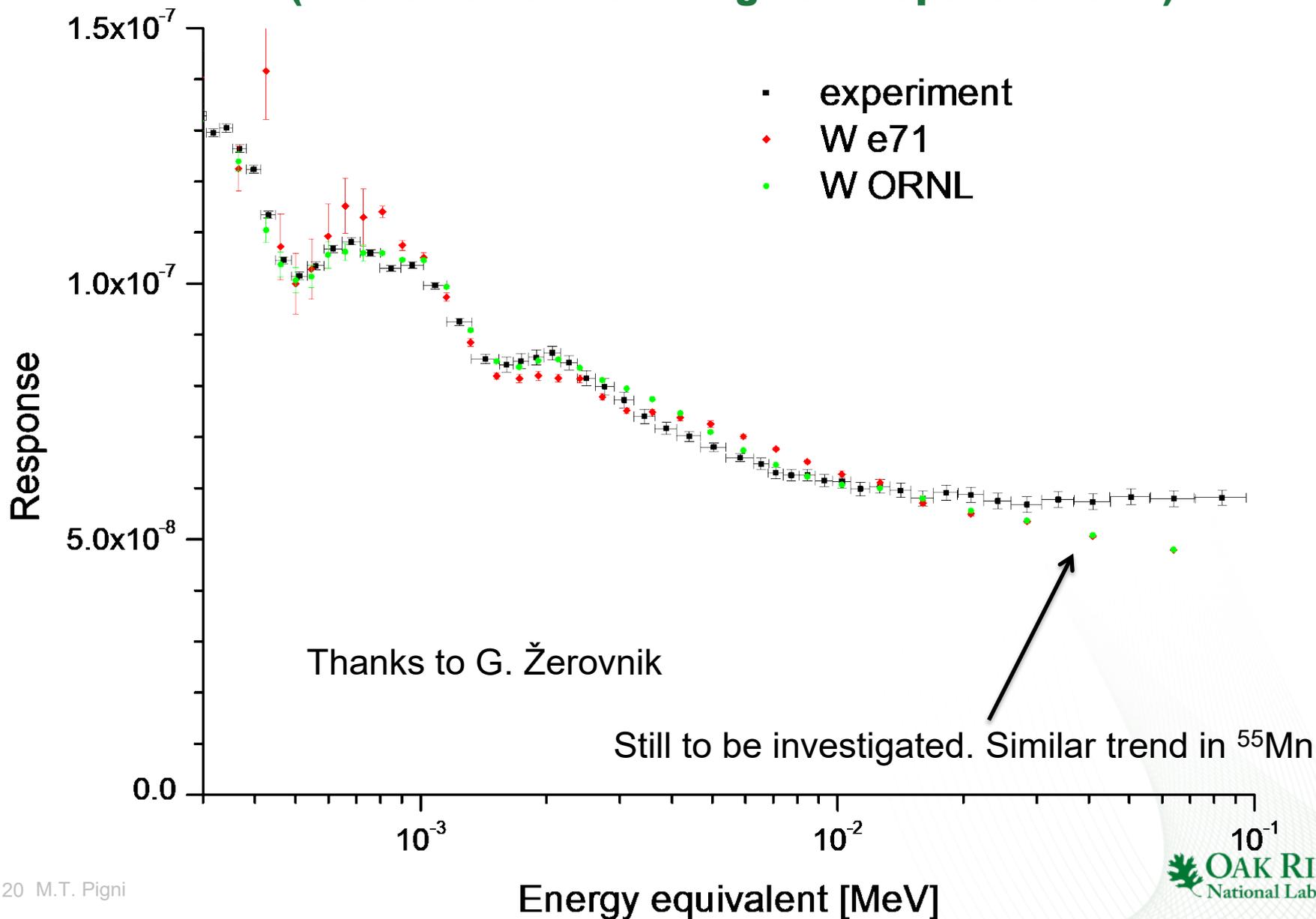
Validation of Tungsten evaluations (2015)

(Grenoble Lead Slowing down Spectrometer)



Validation of Tungsten Evaluations (2015)

(Grenoble Lead Slowing down Spectrometer)



Summary and Conclusions

- We applied the R-matrix SAMMY method using the Reich-Moore approximation to determine a consistent set of neutron resonance parameters and related covariance matrix for ^{40}Ca
- In the analyzed energy range up to 1.5 MeV, the evaluation *triples* the RRR energy range present in the latest US nuclear data library (ENDF/B-VII.1)
- 7 experimental data sets were used to ensure the calculated cross sections were in good agreement with multiple transmission (5) and capture data (2) sets
- Results agree with the systematics of the observed s-, p-, and d-wave resonances, such as level spacing systematics and strength functions
- Charged-particle reaction channels, such as (n,a) and (n,p), were also included in the evaluation
- Calcium evaluated file (LRF=7) also include covariance matrix for the resonance parameters (LCOMP=1)
- **Internal repository (GIT) for all SAMMY inputs and experimental data sets was created within ORNL Gitlab server**
- For tungsten evaluations, the validation analysis on the Grenoble LSD benchmark showed an improved agreement with the experimental response when the new evaluations were included in the ENDF/B-VII.1 library

ACKNOWLEDGMENTS

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Thank you!