Los Alamos NATIONAL LABORATORY

Neutron Evaluations for ENDF/B-VIII.1 beta: CSEWG Evaluation Committee

Mark B. Chadwick
LANL

November 1, 2022

Photonuclear data

- **ENDF7 uses a large collection, many from US (LANL), many more from IAEA late 1990s photonuclear**
  - These are widely used in DOE applications
  - Routinely used in MCNP mission applications by LANL and LLNL

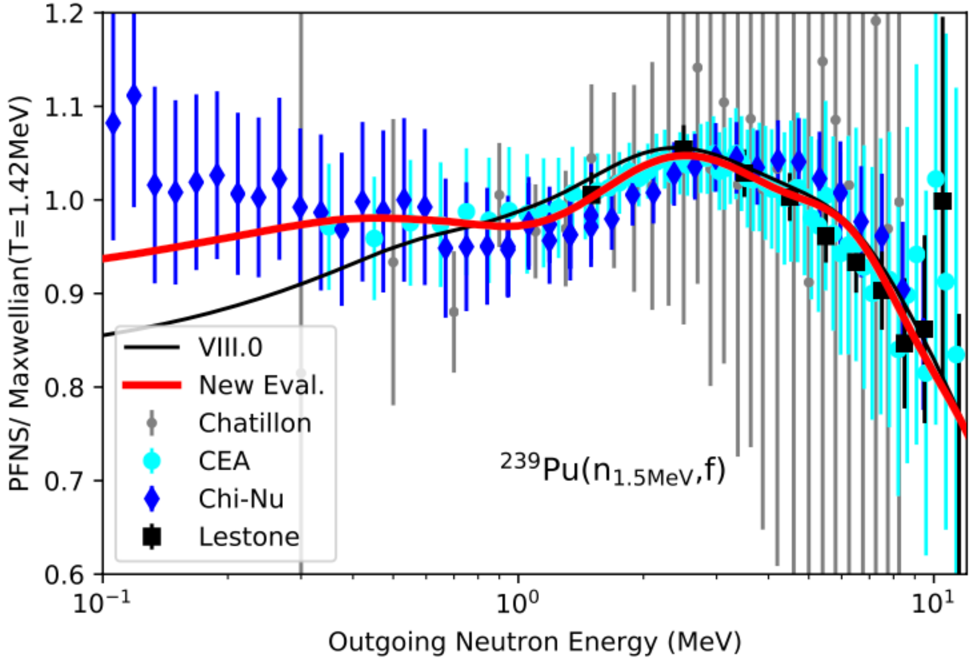
- **New IAEA photonucear library form a few years back**
  - Many/most/all updated
  - US seemed not to submit any evaluations to this project

- **Path forward**
  - Where a new file can be demonstrated to be better, and can be tested adequately, we could update (though do we really want to adopt a totally foreign file)?
  - Beta file = original US files + new IAEA files
  - To adopt a new replacement we should (a) compare cross sections [not done for many, including actinides); test in MCNP applications. See Wim's talk

Overview of My Various Comments Today

- **Comments on FPY radiochemical data and new TUNL data**
  - R-values and impacts if 99Mo has an energy dependence

^{239}Pu PFNS changes from Chi-nu & CEA – a bit softer



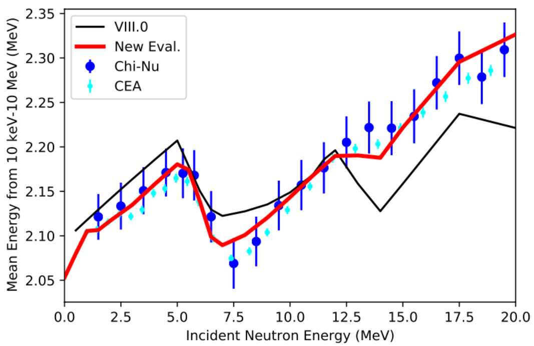
Neudecker evaluation

LANL-LLNL Kelly, Devlin LANSCE.Chi-nu data; & CEA data

These PFNS changes coming are being studied, to assess impacts - OK

PFNS changes have a large impact

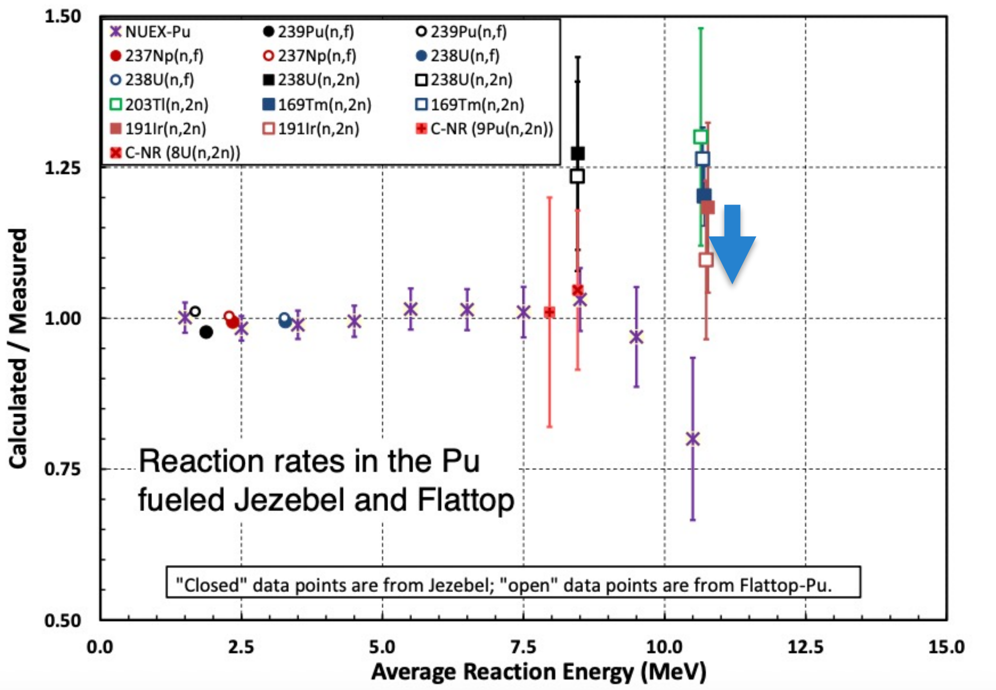
- **^{239}Pu PFNS evaluated to be a bit softer**
  - 20 keV average energy reduction (1%)
  - Informed by new LANSCE Chi-nu & CEA dat



- **This 1% E-av change causes a 120 pcm drop in calculated Jezebel**
  - Other changes reduce the overall drop to ~50 pcm (Jez r5 v. r2)

We have also had insights from LANL fast crits on the PFNS, and perhaps future NCERC experiments could add more insights/constraints

Dosimetry threshold detector testing (Jezebel & Flattop-Pu) to see impacts of new PFNS & other scattering changes

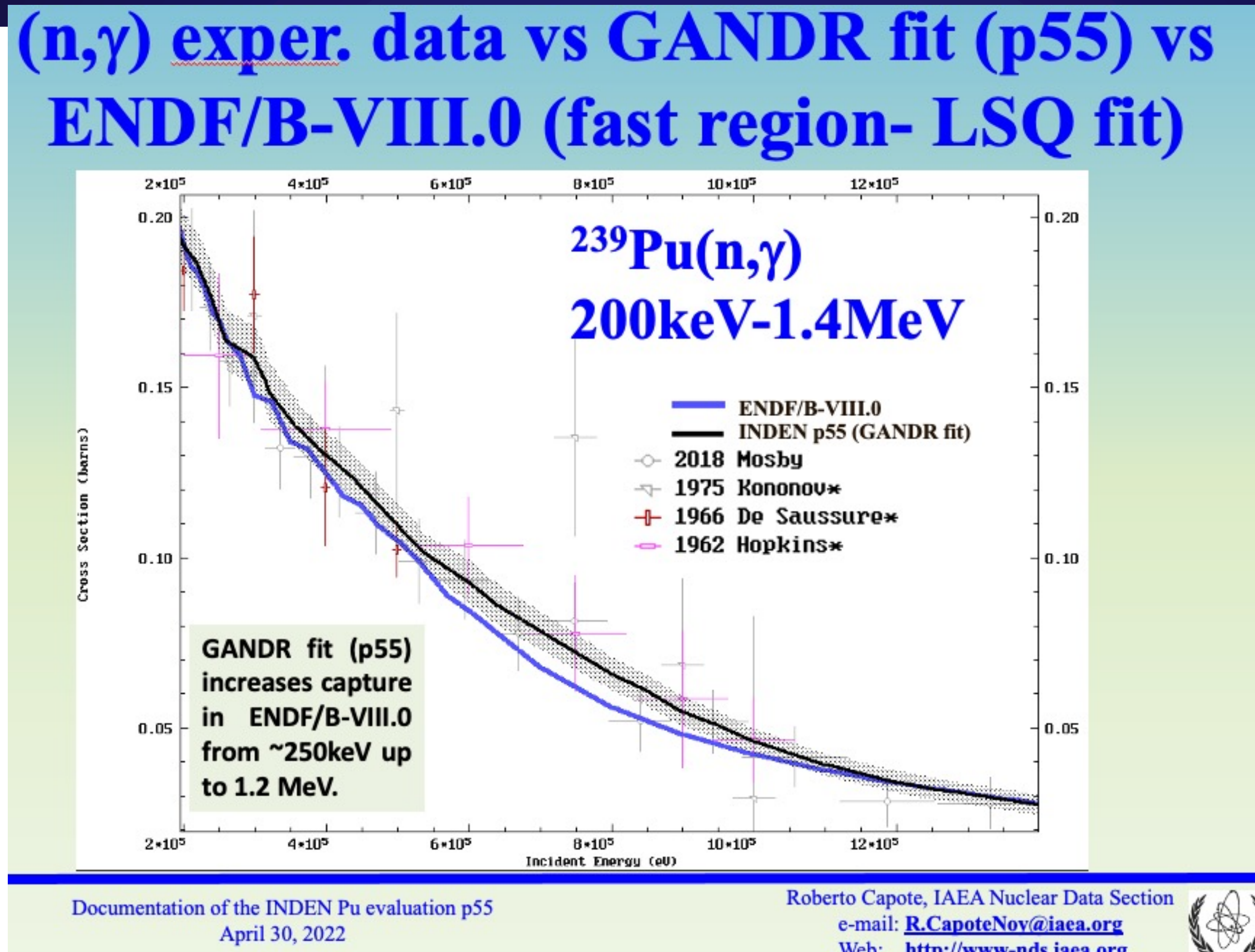


Trkov has already calculated these changes.

XCP5 is now calculating

The previous trend (ENDF8 & earlier) to overpredict higher-threshold n,2n will be reduced. Future NCERC measurements of such threshold detectors would be valuable

New capture is a GLS fit to data using a model prior, and leads to reduced unc. v . 8.0, and better matches Mosby data



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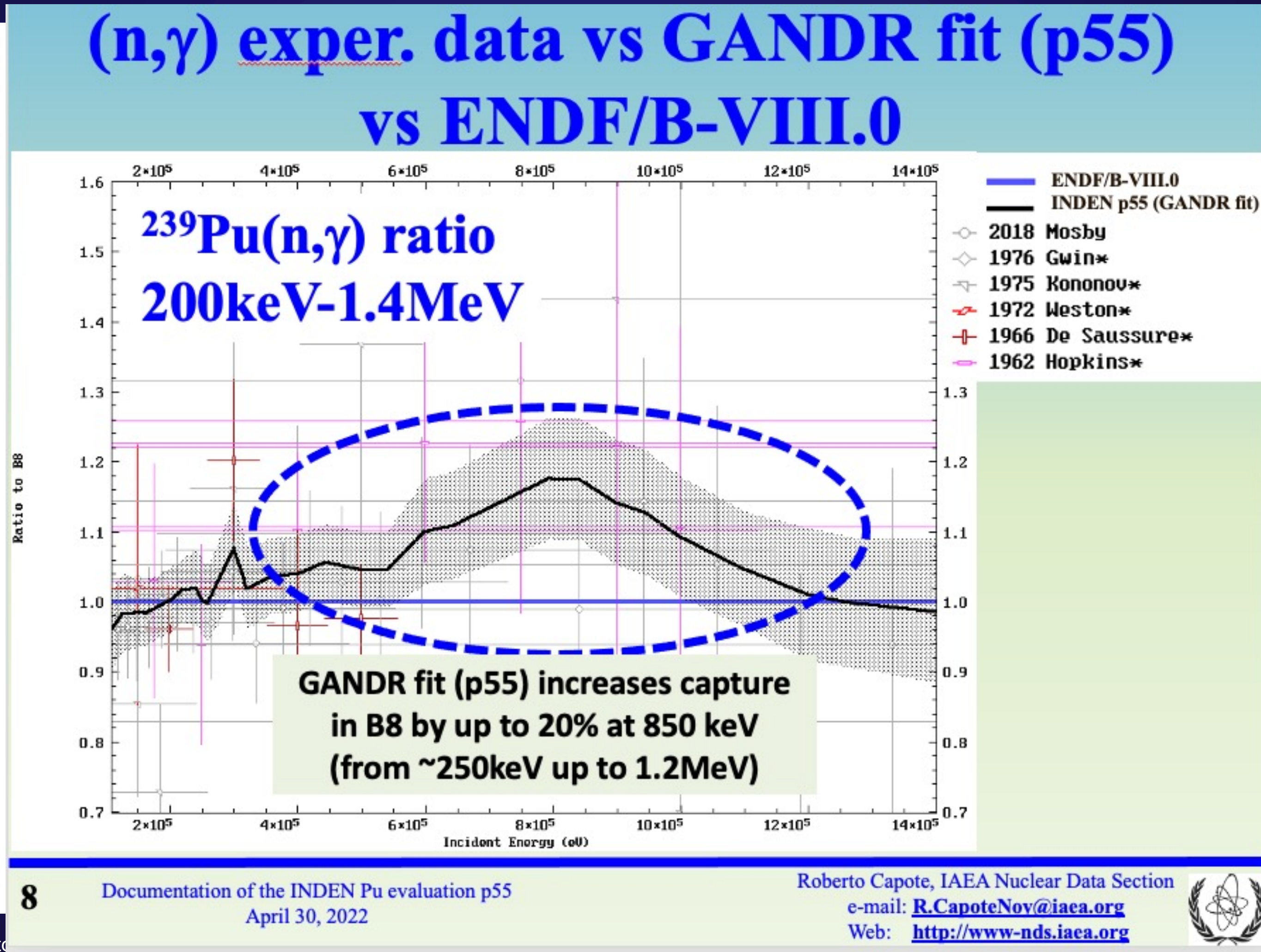
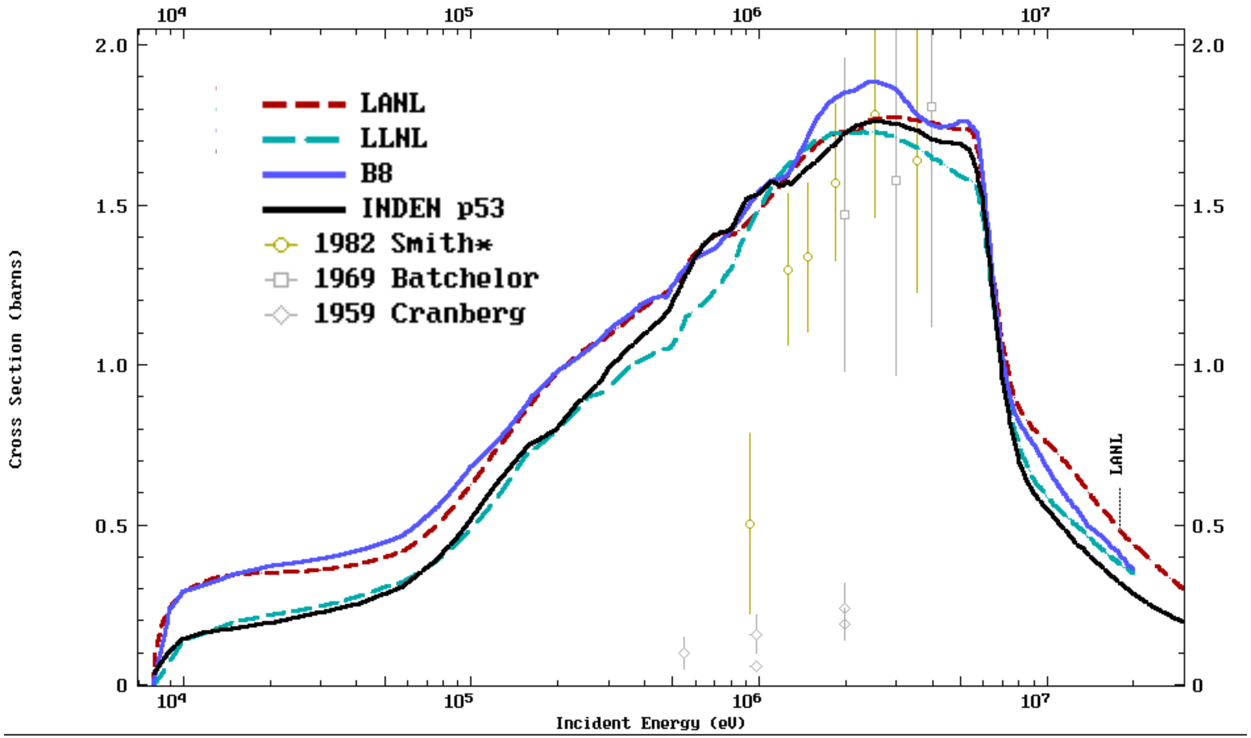


Total inelastic scattering cross sections vs scarce data



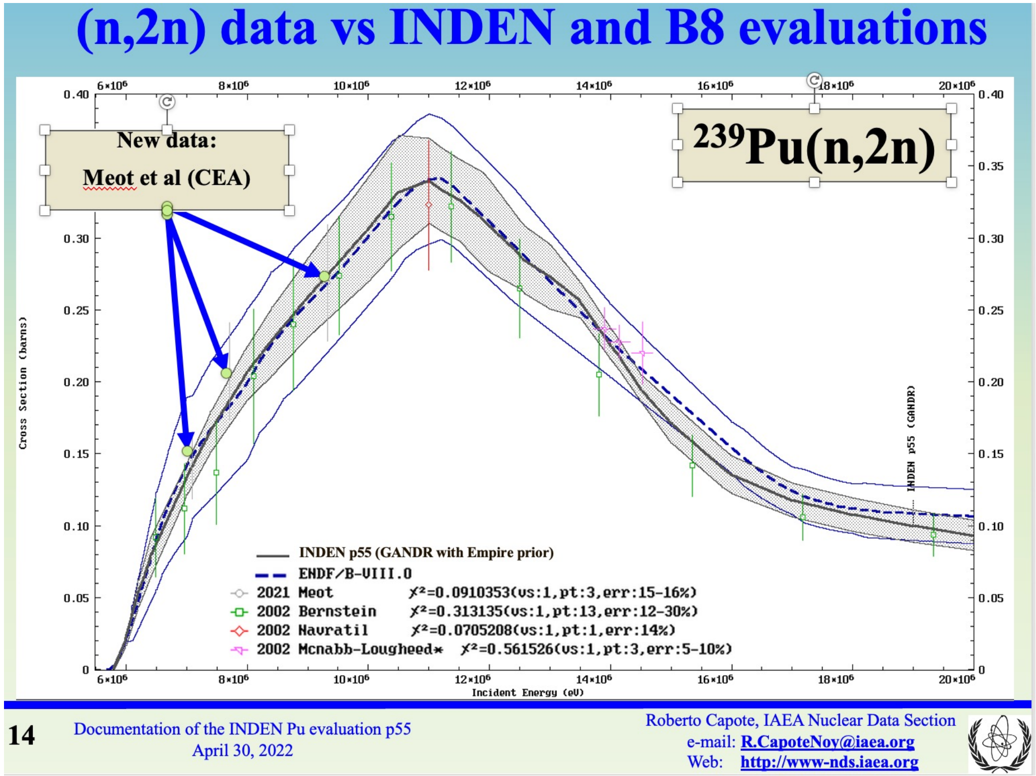
More work is needed to understand best/most accurate result

RPI-type quasi-differential experiments helpful?

Are there NCERC / LANSCE experiments that will help us test and improve our understanding of Pu inelastic and elastic scattering?

Fig provided by IAEA

n,2n – minimal changes versus ENDF8.0. The 7.1-> 8.0 threshold tweak is now replaced by a better treatment, but with ~same result



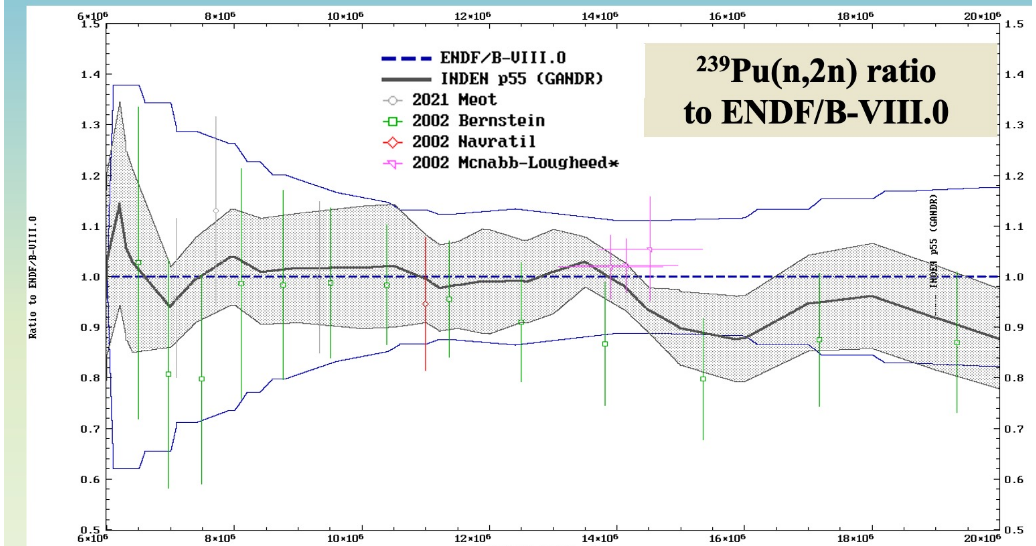
Advantages of Inden.p55

- attractive methodology
- uncertainties well-defined
- uncertainties reduced
- Iterative/small change in mean values v. ENDF8

INDEN-p55 n2n updates the McNabb-Chadwick GEANIE project GLS methodology to add new CEA data & use a calculated prior; result is almost identical to ENDF8.0

n,2n – ratio plot shows the uncertainty reduction

Ratio of (n2n) data and evals to ENDF/B-VIII.0



Excellent agreement with B8, improvement is seen relative to B8 above 15 MeV in INDEN eval. Evaluated uncertainty is reduced due to the combined model+data fit.

15 Documentation of the INDEN Pu evaluation p55
April 30, 2022

Roberto Capote, IAEA Nuclear Data Section
e-mail: R.CapoteNoy@iaea.org
Web: http://www-nds.iaea.org

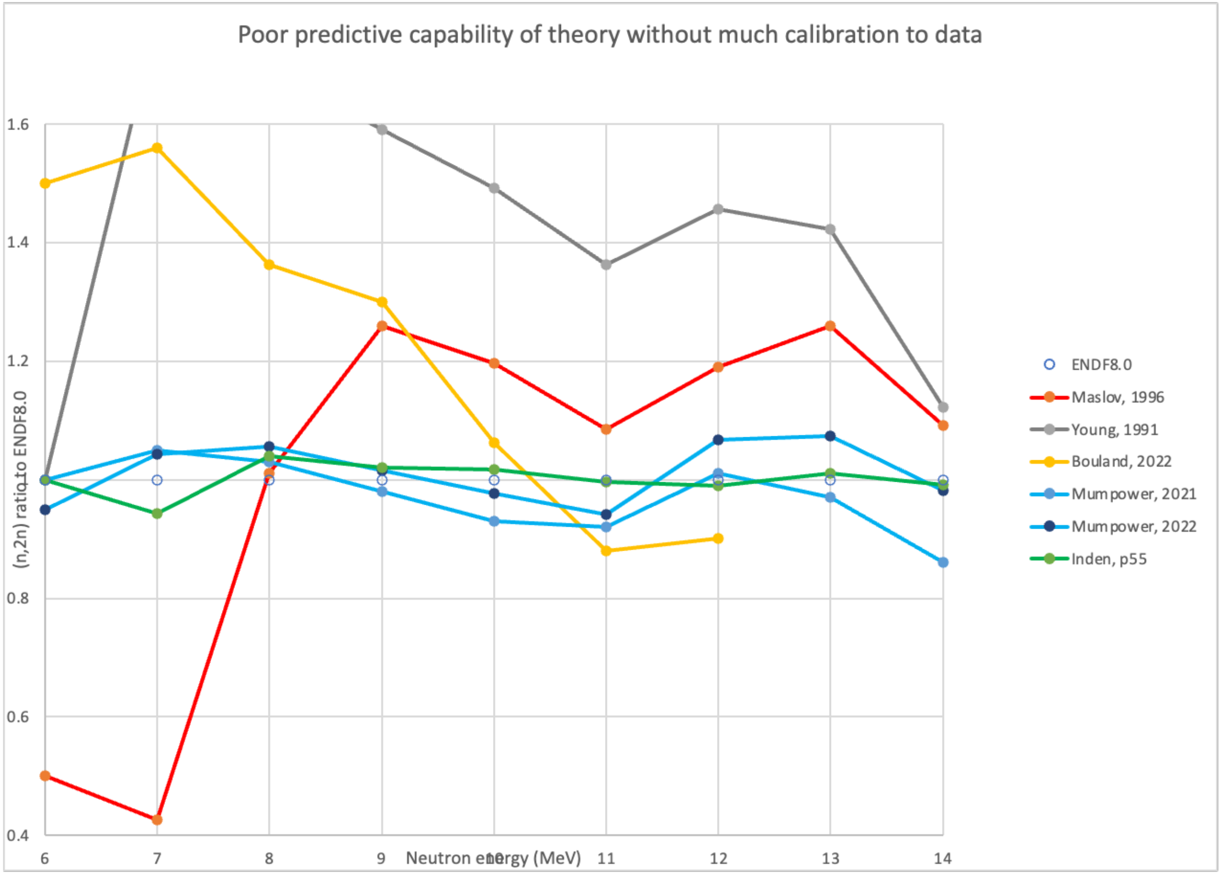
^{239}Pu(n,2n) is ~unchanged, but some small impacts seen

- **In a Jezebel fission spectrum the calculated n,2n conversion rate is reduced by 2% versus ENDF8.0**
  - This is because the 239Pu PFNS is slightly softer
  - It is still 4% more than ENDF7 because of the threshold rise change

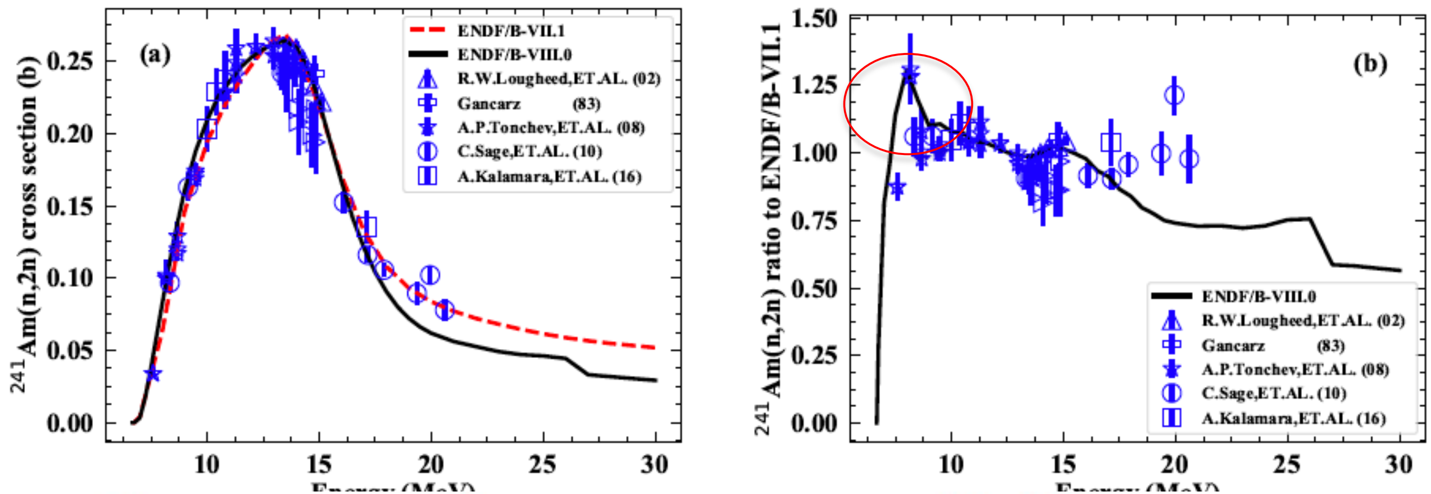
- **At 14 MeV, the n2n is ~the same as ENDF8.0**
  - effect of change is like for ENDF8

Larger changes in (n,2n) are unwarranted at this time. The 8.1 beta file is a GLS fit to the data using a model prior, and has the lowest Chi-2.
Model calculations are not accurate enough to warrant “overriding” this exp-based approach. See for example other cases, ^{241}Am(n,2n)

Theory prediction capability for 239Pu n,2n is not high (but theory can be calibrated to measurements - but even then the model is not as accurate as a data-based approach)



241Am(n,2n). ENDF8.0 model calibrated to data gives a rise from threshold that is too high. We would like to change this for 8.1



E_{inc} range	χ^2		weighted C/E	
	ENDF/B-VII.1	ENDF/B-VIII.0	ENDF/B-VII.1	ENDF/B-VIII.0
All	2.917	4.984	-0.00244	0.0210
7.5 – 10 MeV	4.709	11.859	-0.0279	0.107
< 11 MeV	3.907	8.612	-0.0335	0.0735
11 – 15 MeV	2.266	1.624	0.0124	0.0158

Table 1: χ^2 and weighted C/E values for the ENDF/B-VII.1 and ENDF/B-VIII.0 libraries compared to experimental data.

Amy Lovell

Fission Product Yields- Chadwick comments

- Looking forward to seeing details
- Please provide summaries of where new FPY evaluations differ more than say 1-sigma from current FPY Engalnd and Rider (their 1-sigma) to guide and focus discussions of changes
- The NNSA labs are esp interested in Mo, Nd, Zr, Cs, …

Fission Product Yields

- **Next slides give input to the CSEWG FPY subcommittee**
- **It concerns FPYs derived form LANL radiochemical R-values, Q-values, and K-factors**
- **Focus: What is the impact pf the new TUNL-LLNL-LANL data on LANL FPYs derived from these radiochemical data, esp. 99Mo?**

FPY energy dependences

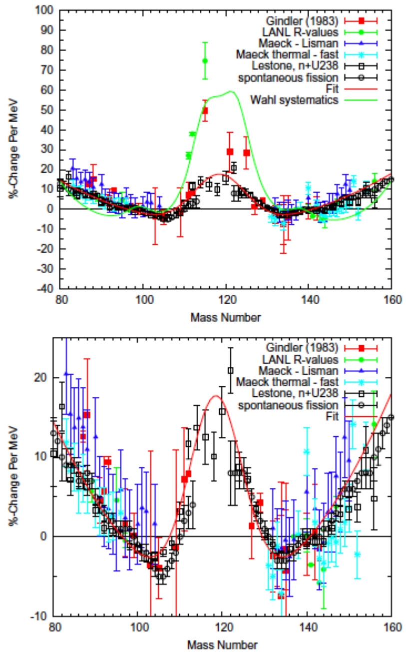
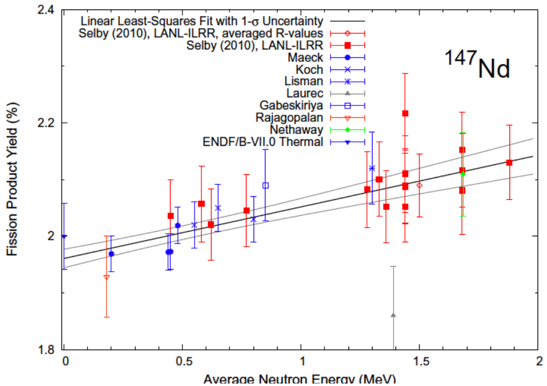
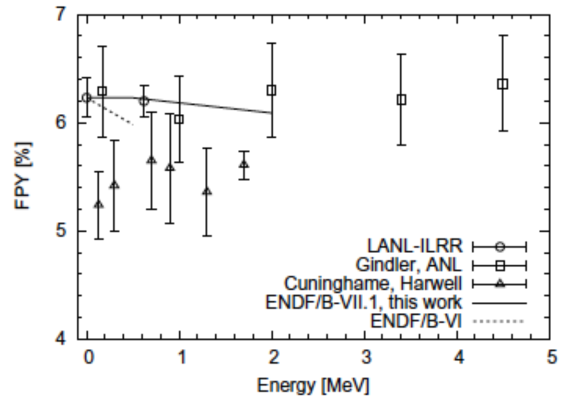


FIG. 10: Energy dependence of n+^{239}Pu FPYs in the 0.5 to 2 MeV region, inferred from various sources of data described in the text. The lower panel is magnified to better show the variations.





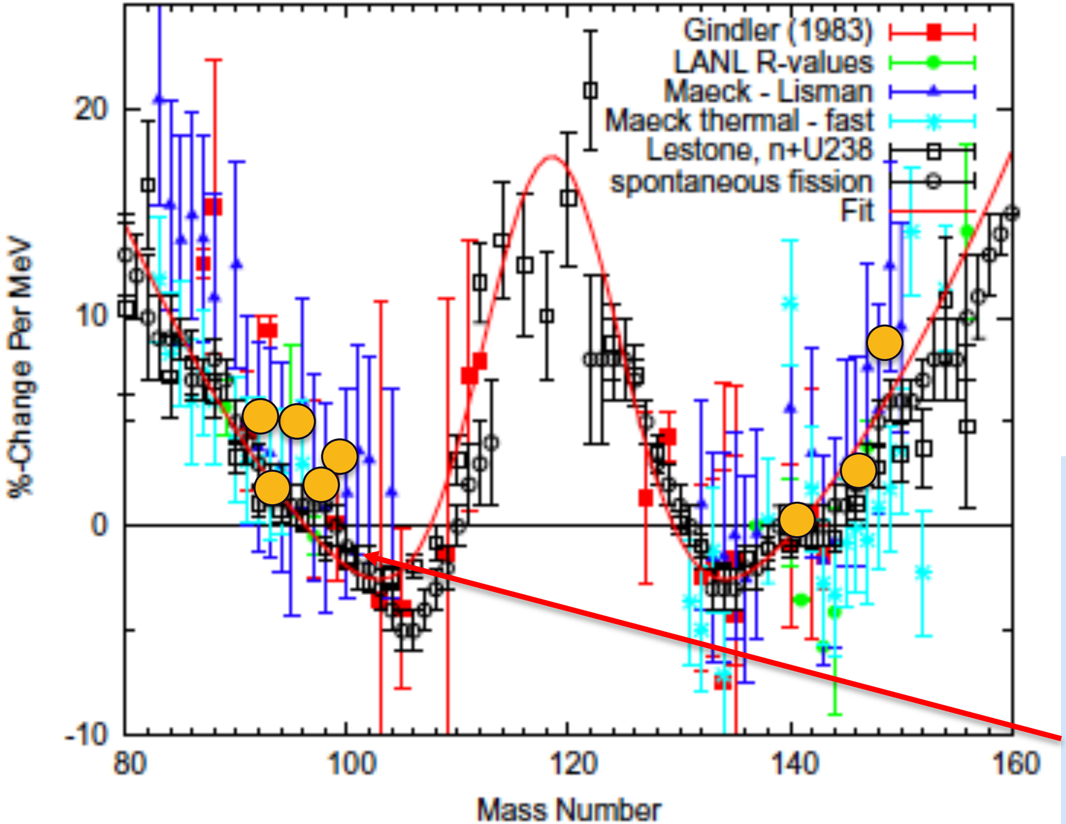


FIG. 10: Energy dependence of n+^{239}Pu FPYs in the 0.5 to 2 MeV region, inferred from various sources of data described in the text. The lower panel is magnified to better show the variations.

Tonchev et al, 2022
Simple estimate from TUNL data below 2 MeV

See fig 10 p2944. One sees energy dependence's for 99:
- Gindler - zero
- lestone u8 and spent fission - negative
- above. Slightly negative
- Maeck-lisman positive with big unc?
- new TUNL. Positive. First points have about +2.9% per MeV.

ENDF8: Current p2947 trend from 0.5 to 2 is 6.23 to 6.09

ie % drop of 2.3% or per MeV drop of -1.5% per MeV.

FPY energy dependences

index	FPY	Unc. [%]	Reference
1	6.08	5	Rajagopalan [53]
2	6.35	3.2	Yurova [55]
3	5.91	5.2	Larsen [44]
4	5.98	5	Laurec, CEA [38], unc. increased
5	6.23	3	Gindler [48]
6	6.209	1.3	Maeck [37]
7	6.285	1.3	Lisman [36]
8	6.22	1.6	Meta-analysis (this work)
9	6.20	2.4	Selby [1], LANL-ILRR
Av.=	6.23	0.7	nominal av. energy 0.5 MeV

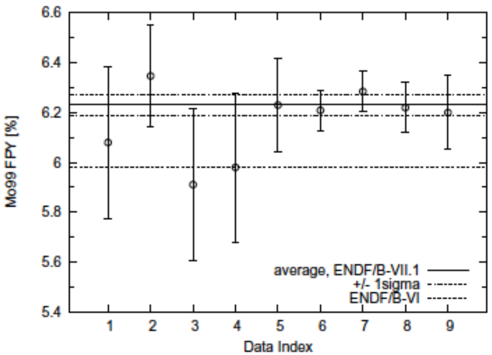


FIG. 13: Evaluated ^{99}Mo FPY for fission-spectrum n+^{239}Pu, and comparisons with other analyses, experimental data, and evaluated values.

If we concluded that there is definitive evidence and a strong basis to have a 99 energy dependence, what is impact?

R-values unchanged. That's their beauty,

If we concluded in a positive 99Mo FPY energy dependence in Pu (0-2 MeV):

Q99 would have to be updated.

Presently we use 1.015 for all neutron energies. We would have an energy dependent Q value above 0.5, up to 2 MeV

FPYs: using Y^i-fast^{Pu} = Y^i-th(^{U235}).Q99(E). R^{Pu}

Q99(E) would start at 1.015 at 0.5 MeV, and then change, leading to modified FPYs

If ^{99}Mo had a positive energy dependence from 0.5-2 MeV, then LANL RC FPYs would increase (and #F decrease). (Visa-versa if negative energy dep.)

99Mo FPY energy dependence in the 0-2 MeV region

Los Alamos radiochemical & fission chamber data, See Selby et al., from thermal to ~0.5 MeV
~ small & negative (-1% per MeV)
~ ignored (ie 0 assumed) converting Rs to FPYs

Q99 fast = 2.445 (K u5 thermal)/2.409 (K pu fast) = 1.015. See table xiii and xc page 2904
Q99 thermal = 2.445/ 2.396 (K pu th) see table xiii VII = 1.020
Ie slight negative trend. (-1% per MeV)

Gindler ANL data
~0 (none)

New TUNL data
~ 3% per MeV
Positive energy dependence

Should the 99Mo energy dependence be updated, when converting Rs to FPYs (currently assumed to be zero). Maybe or maybe not.

Some next steps on this question of whether or not to update FPYs from LANL radiochemical measurements

- **Evaluate the 99Mo FPY (and therefore Q99) energy dependence based on all info we have**
  - Ask LANL-LLNL-TUNL to provide unc. on the relative values (ie shape) of their FPY data (esp 99Mo, 147Nd). (Done, MBC-> Wilhelmy)
  - Consider whether we also fold this TUNL energy-dependence over critical assembly spectra to enable more direct comparisons to our LANL data
  - Assess if the uncertainties are sufficiently different from a currently assumed energy trend of zero to warrant a change

- **Engage RC experts at LANL and LLNL for feedback**

- **Provide a recommendation to CSEWG**

Backup

Principles driving our ENDF file goals

- **Should be most accurate representation of reality**
  - Optimally match experimental data
  - Use theory and modeling to augment use of data
  - Benefit from collegial peer-review expert discussions
  - Ideally have updated covariances that show smaller unc. [reflecting progress!] and are credible

- **Integral data testing *(e.g.* k-eff) is important in validation & assessment**
  - While very import, this doesn’t supersede the above “fundamental data” accuracy requirements

- **Should use methods that have been established as “best practices”**
  - Although the ^{239}Pu reactions are not ”standards”, they are tremendously important and it is appropriate to look to approaches developed in the standards community, and other “high accuracy” communities, *e.g.* reactor dosimetry data
  - Covariances (ideally) obtained form the same evaluation methodology that created the eval.
  - We should strive not to use the integral k-eff data as a guide to individual cross sections evaluation – they should be based on the fundamental data. (typically only do a nubar tweak at end to optimize keff)
  - Only make changes/updates when there is a compelling reason to do so
  - Only make changes after impacts have been assessed by our users
  - Document the methods and the evaluation results

Agreed-upon common elements

- **I suggest**
  - Resonance and thermal eval. (from ORNL, RPI, IAEA)
  - Fission PFNS and nubar (from LANL, informed by LANL-LLNL, CEA data)
  - Fission cross section (from LANL & IAEA standards team)

- **Others?**

Some evaluation “best practice methodologies”

- **Approach of using a model prior with a Bayesian update & GLS data fit is widely used for most accurate data evaluation**
  - “Best of both worlds” – use of experimental data & model calc
  - Established in standards and IRDF2 community.
  - *Don Smith: “it has been contemporary practice for most of the evaluation efforts aimed at generating content for the ENDF/B library to be undertaken using Bayesian evaluation techniques, mainly those that involve the generalized least-square (GLS) method. There is widespread agreement in the contemporary nuclear data evaluation community that this approach is preferred since it is based on well-established and accepted procedures from mathematical statistics.”*
  - *Pat Griffin: “rigorous evaluation: with the model prior and GLS adjustment process”.*
  - But less useful when there are very few data, e.g. Pu inelastic scattering
- **Model fitting approach**
  - It has been very common to do evaluations in which one performed a global model calculation using a comprehensive modeling tool; and make model parameter choices that “fit” measurements (often somewhat informally, not using LS)
  - this approach has been adequate for many applications
  - But it suffers from
    - models being “too stiff”
    - doesn’t use experimental data in a rigorous way (eg Bayesian)

Feedback from last summer's review

Suggested priorities for the coming months

1. **Inelastic and elastic scattering, especially for incident energies below a few MeV.** All 3 teams – compare theory/methods and compare against experimental data, to understand current differences, and to build case for which approach is preferred. Currently, it is roughly the case that LANL and ENDF/B-VIII.0 are similar, and LLNL and INDEN are similar. Ian Thompson has shown that the differences are biggest for the first inelastic level, and that it is likely the compound inelastic contribution that differs most.
2. **14 MeV inelastic and preequilibrium.** Further optimization to best match against (n,xn) and Livermore pulsed sphere data would be useful. LANL is a little high, and LLNL a little low. On the theory side, the treatment of the direct inelastic and pre-equilibrium components is probably the most striking difference between the evaluations. It would be interesting to better understand how those choices impact the result for Kammerdiener for instance, and how sensitive those results are to wiggles in the parameters.
3. **Fission cross section.** The INDEN/LANL approach that uses the standards work should continue to be refined as the standards effort continues. This team should collaborate with LLNL to understand differences compared to LLNL's independent study, and to see if we all agree on how TPC impacts the new results.
4. **Fission nubar.** The results used by LANL and INDEN, coming from an analysis of measured data as well as from broader fission model calculations, could be usefully studied more, so as to justify this approach's results (leading to an evaluation somewhat above the nubar data for energies < 1 MeV). Explain the validation basis for this approach. Why do we believe it over just using the data?
5. **PFNS.** The present upgrade from LANL used in LANL and INDEN, informed by the new Chi-nu and CEA data, seems well founded. LLNL should consider adopting this.
6. **Capture:** LLNL and LANL may want to consider using a generalized-least-squared measurement-based approach more like INDEN's. Discussions, between the three teams, of assessed uncertainties on individual measurements is worthwhile.
7. **n2n.** All approaches give fairly similar results. We will be providing feedback from some of our users on the impacts of different choices here.
8. **Resonances.** INDEN (ORNL/IAEA) should continue to refine their work.
9. **Data ambiguities?** Ensure that we are comparing those evaluations to the same data sets. For instance, Mosby's capture data is surprisingly not in EXFOR yet. Hopefully everyone is using the same data set, but let's check, for capture, n2n etc In that vein, we could also encourage every team to calculate a chi^2/d.o.f. value for their evaluation against (some) data.
10. **Calibration to Jezebel r2 or r4? K-eff** We – and all 3 teams - should all discuss this. In favor of r4: it's the latest work from Jeff Favorite and no simple way to discount it. In favor of r2: we could punt on making a change until ENDF-9, and at this stage maintain continuity by sticking to r2. Our decision will also be informed by suites of validation testing from our user community.
11. **Covariances.** These need to be developed, and we will engage the help of the CSEWG covariance and validation committees for feedback. INDEN has new covariances for both n2n and capture and these show notable uncertainty-reductions compared to 8.0. Some

Summary of SME input from the summer review

Summary, where I include entries if the reviewer communicated explicitly-positive views on a certain reaction channel in an evaluation.

	Inel.	Inel 14 MeV	n,g	n,2n	n,f	nu	pfns	RR	thermal	Current File maturity
Brown	LL		IN	IN	IN, LA, LL		IN, LA	IN, (LA)	IN, (LA)	IN
Carlson			IN		IN, LA, LL				IN, (LA)	
Chadwick	IN, LA, LL	IN	IN	IN	IN, LA	IN, LA	IN, LA	IN, (LA)	IN, (LA)	IN
Hilaire										
Koning	IN	IN	IN	IN	IN, LA	IN, LA	IN, (LA)	IN, (LA)	IN, (LA)	IN
Talou	IN, LA, LL	IN, LA, LL	IN, LA	IN, LA, LL	IN, LA, LL	IN, LA	IN, LA	IN, (LA)	IN, (LA)	
Lestone				IN, LA, LL			IN, LA, LL			
Thompson	IN, LA, LL		IN	IN, LA, LL	IN, LA, LL					

IN = INDEN/LANL
LA=LANL, and (LA) is used for a case where LANL adopts the new low energy ORNL-INDEN RR.
LL=LLNL

See documentation compilation sent out from the previous review.

Additional feedback welcomed after today.

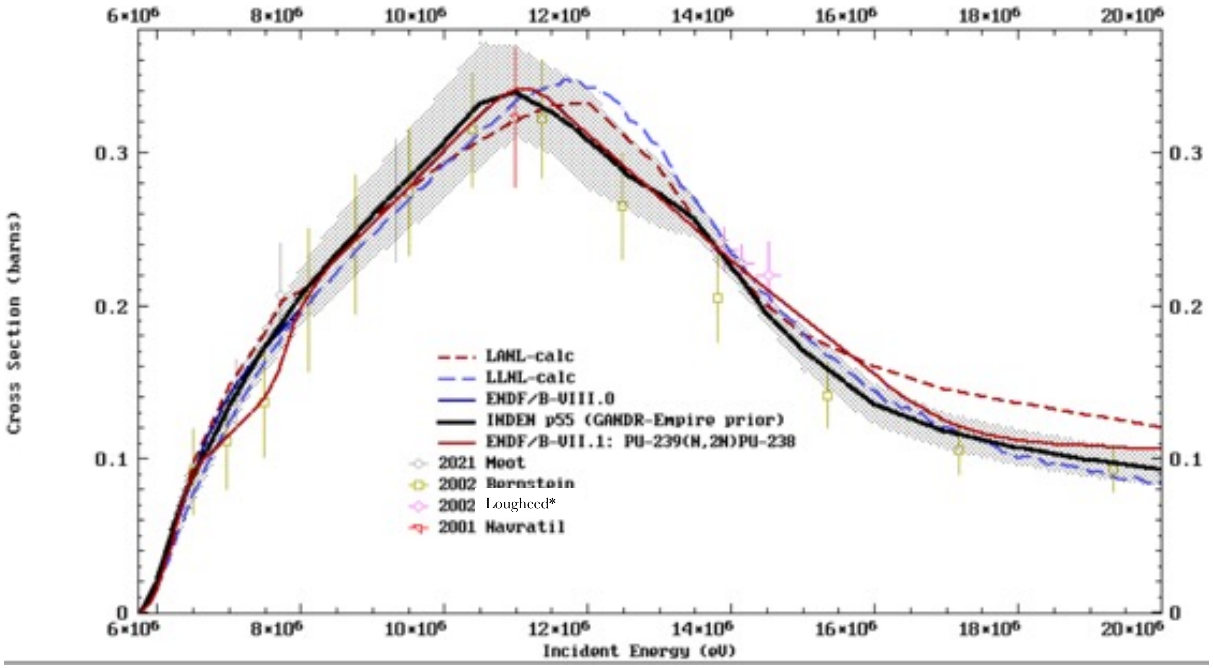
We also have additional input from McNabb on our previous SME list, & Don Smith & Pat Griffin as other evaluation SMEs

Summary of Chi2 (sum of the tabulated Chi2 in the attached figures divided by the number of data sets, 12 for capture, 4 for (n,2n))

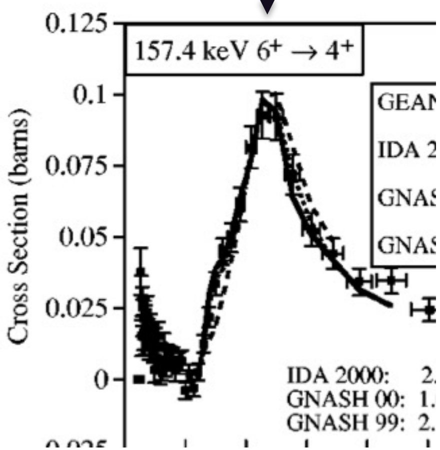
	Capture	(n,2n)
LANL	9.1	0.45
LLNL	10.3	0.26
INDEN	2.1	0.24 for p53, p54a=0.20 p55=0.26
ENDF/B-VIII.0	4.2	0.24

Example of model prediction limitations: n,2n

- **Calculations – even “very good calculations” differ by 10-20%. Need ”calibration” to agree with Lougheed at 14 MeV**

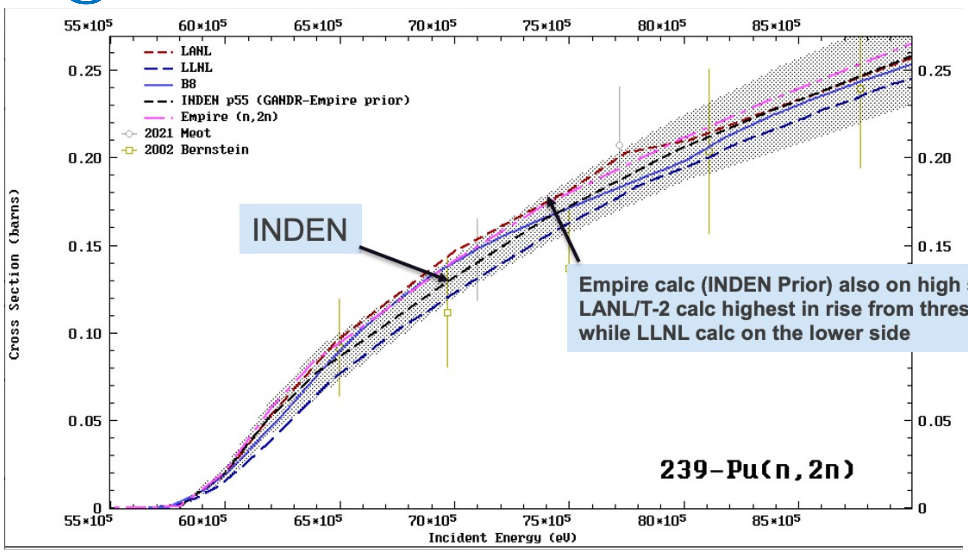


Also, some calcs get the peak at too high an energy (GEANIE observes it at 11.3 MeV), see Bernstein data



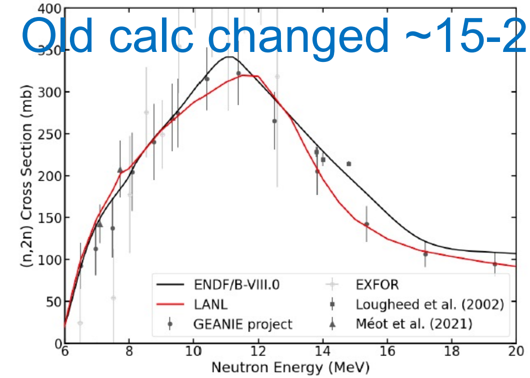
It's not credible to argue n2n calculations alone are accurate to << 15%

LLNL & LANL Calcs differ by ~20% @ 7 MeV

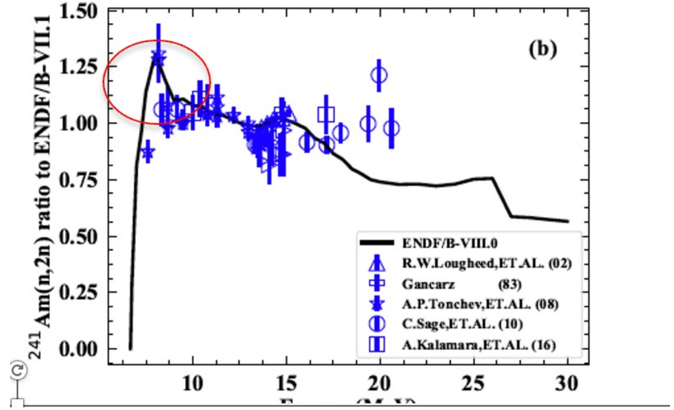


Empire calc (INDEN Prior) also on high side
LANL/T-2 calc highest in rise from threshold, while LLNL calc on the lower side

Old calc changed ~15-20%



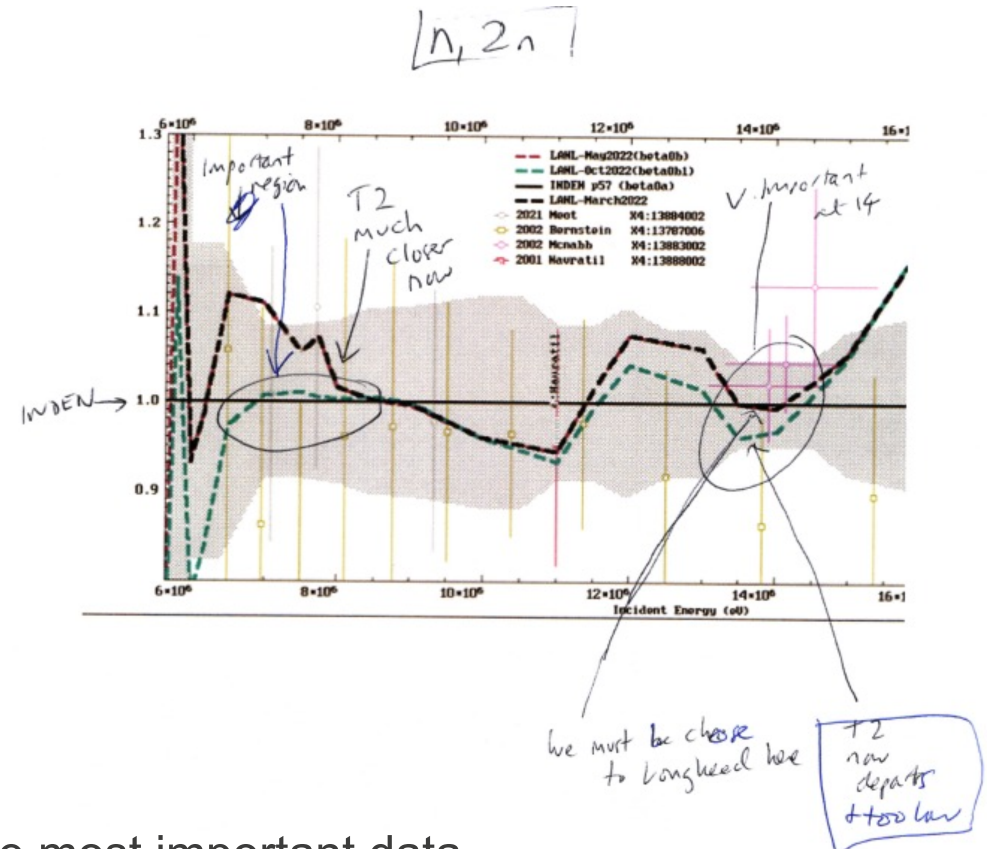
^{241}Am n2n calc. ~10% high 7.5-10 MeV



Hence the advantage of using a model prior with subsequent GLS fit of data

More SME review feedback

N2n review feedback – convergence (partially) of T2 to INDEN but now T2 undercalculating important 14 MeV region



Lougheed is the most important data

N2n review feedback: Pat Griffin, SN expert in n2n dosimetry

Summary of review comments on 239Pu (n,2n), Pat Griffin, SNL, Oct 18, 2022

General comments on methodology. The rigorous INDEN evaluation, with the model prior and GLS adjustment process, is clearly the preferred evaluation. The covariance should represent the method used in the evaluation. This is a very strong point for the INDEN evaluation. Methods should include fitting the data using a least-squares approach that includes the influence of the energy-dependent correlations in the calculated prior.

INDEN: The INDEN evaluation [with model-based prior including a high-quality covariance matrix and with the GLS adjustment] is excellent for the (n,2n) reaction. If this was a single reaction evaluation for a dosimetry file, there is no question but this would be the recommended evaluation. The rigorous INDEN evaluation, with the model prior and GLS adjustment process, is clearly the preferred evaluation. It is a bonus that the INDEN evaluation provides a better (the best – by definition of the least squares adjustment) fit to the data – as evidenced by the experimental-based chi-squared metric. And the INDEN evaluation does not show kinks or shape artifacts that would cause me to question the prior or the adjustment.

The GANDR GLS chi-squared per degree of freedom is very close to the data-only metric reported – and confirms that the chi-squared is dominated by the data and not the prior correlation matrix. Regarding the statement "The INDEN GLS-evaluation approach was not constrained by data from other channels except in one regard: the EMPIRE prior was a model calculation that included all channels (analogous to the T2 CoH model calc). The only two channels that were fitted directly to experimental data using GANDR (in the GLSQ fit) were capture and n2n. Those two channels are practically uncorrelated (capture is already negligible once the n2n opens)." I repeat this comment in this summary, to emphasize that this is an important question and that the answer had to have visibility. And this answer is sufficient to remove any concerns regarding this issue.

T2. It should involve fitting the data using a least-squares approach. The use of an eyeball metric [i.e., not using LS] rather than a rigorous/objective minimization approach in the T2 evaluation is not good. And the difference in these two chi-squared shows the importance of a rigorous LS process. The series of "model adjustments" to address issues in the T-2 evaluation has me concerned. I can understand why this was attempted/done in the T-2 evaluation – but the tendency to "improve/change" model approaches until you get a good match is not what I want to see. The kink at 8 MeV clearly raises questions. The INDEN evaluation does not show kinks or shape artifacts that would cause me to question the prior or the adjustment.

n,2n review feedback: Dennis McNabb LLNL and Chadwick (SME reviewers)

^{239}Pu (n,2n) for the next ENDF release

M.B. Chadwick and D.P. McNabb
LANL & LLNL
October 2022

Abstract. We recommend the IAEA's INDEN 239Pu(n,2n) evaluation be adopted in the next ENDF release. It involves generally-small changes compared to the previous LANL-LLNL ENDF8 and ENDF7 evaluations, but changes that are warranted based on new data and methods. It builds on the data-driven approach used in the original LLNL-LANL 2001 (n,2n) evaluation adopted for ENDF7, adding in recent data measured by the CEA (Meot et al). It uses a methodology that has been used by the IRDFF-II (International Reactor Dosimetry File) community, involving a generalized least squares (GLS) fit to the data with use of a model calculation as a prior, using the validated GLS code GANDR. Uncertainties are obtained consistently within this methodology and show an uncertainty reduction in the rise-from-threshold region compared to the previous evaluations.

n,2n review feedback: John Lestone SME reviewer

John Lestone, LANL, 23rd October 2022

(1) Pu PFNS
My review focuses on a comparison of the proposed evaluations to my previously inferred Pu PFNS experimental data obtained via UGT Nuex data. The new evaluations compare well to the Pu Nuex inference with matches of a quantity similar to past evaluations. The Pu Nuex inference was for fission neutron energies > 1MeV, and needed to be slightly renormalized given recent changes (shifts) in the evaluated PFNS below 1 MeV. The new Neudecker evaluations are a little softer than ENDF VIII, and a marginally poorer match to the Pu Nuex data than that previously adopted by ENDF VIII, but well within the Nuex uncertainty estimates, and appear to be a good compromise between the NUEX analysis and the more recent experimental observation made at LANSCE by LANL/LLNL and CEA teams. I previously sent an email on this in the summer, with a figure, so here I have just repeated that assessment.

(2) Bayesian methods
For nuclear data evaluation in cases with sparse experiment data sets, I have a preference (bias) for Bayesian based approaches, and lean towards methods with model priors obtained via an array of theoretical calculations, with these priors updated with the available experimental data. I also point out that standard chi-squared analysis is Bayesian analysis in the limit of independent Gaussian uncertainties and is in many case "good enough."

(2a) Pu(n,2n)
I lean towards the INDEN evaluation because of its more rigorous approach in defining priors based on theoretical models and then updating this information with experimental data using a least squared approach. In some cases least-squared approaches are a good substitute for chi-squared analysis.
I have previously modeled (n,2n), and (n,3n) reactions with various theoretical approaches and found one must consider the possibility that one's beloved model could give cross sections that are off by ~20%. These uncertainties are associated with model parameters that can alter the competition between fission and neutron emission, due to uncertainties in fission barrier heights (both inner and outer barriers), the calculated excitation energy dependence of single particle level densities, and the inclusion of rotational band structures. All these uncertainties highlight the need to update theoretical model priors by experimental data. As an example, in my own evaluation of Pu(n,2n) my theory based model prior needed to be significantly modified by the Lougheed experimental data points near 14 MeV. I found the calculational approaches by LANL (T-2) and LLNL, with an informal calibration to match certain data, less rigorous then the INDEN methodology.

Dear David

Just a few comments about yesterday's meeting.

(1) I heard Mumpower use arguments: that because another theoretical calculation agrees with theirs, this adds confidence that theirs is OK. Such statements should get very little weight.
(2) Too much speculation about experimental results being incorrect. Obviously discrepant sets alert us to problems. But when there is only one set in a given region these data should get a strong weight.
This is the case for n,2n questions. Speculation about the incorrectness of n,2n experimental cross sections > 15 MeV should get little weight without proof. I like to think about what future evaluators will think to help guide decisions.
For example for n,2n at high energies, if we go with data, but theory is shown to be better via future measurements (or additional analysis) then future evaluators will be kind and understanding.
However, if we use models to over-ride data, and later it turns out that the experimental data is correct, then future evaluators would have a negative view of our decision processes.
(3) I think ENDFs first focus is primary data. Integral data like the critical bench marks are important cross checks but not the main guide.
(4) So with a focus in the primary data, I believe one of the evaluations is the better. I believe the review process as a whole should be asking similar questions. I was hoping to discuss with other reviewers to help determine if my view is valid. Thus I was hoping to see if there was consensus amongst the reviewers.
But yesterday's meeting with all three teams present (but one underrepresented) could only lead to a consensus view at the expense of the better evaluation.

Sincerely
John Lestone

Capture

INDEN's is preferred because

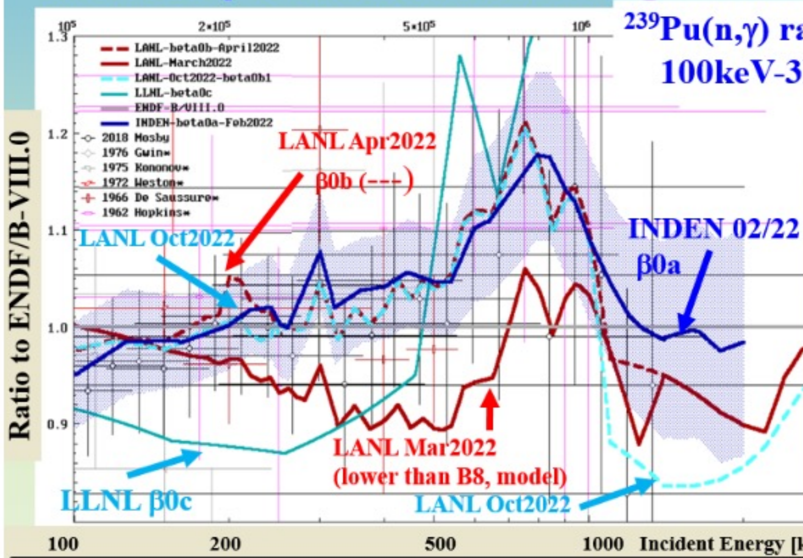
- **It uses a well defined methodology** – GANDR using GLS with a model shape prior. Uses experimental uncertainties
- Has lowest chi-2, 1.6; (T-2=5.2, ENDF/B8.0=3.0)
- Includes 12 data sets, updated using new standard fission xs, via alpha=c/f – LANL data very influential (Mosy and older/updated Hopkins)
- **Priority:** they were the *first* to provide an improvement over 8.0, especially in the fast region, and they were the first to be articulating that ENDF8 was too low above 0.5 MeV – including base don LANL Mosby data

T-2 file concerns

- **Early May file unjustified methodology**, though by the evaluation became similar to INDEN's. *Doesn't use experimental uncertainties* – and it uses weightings that vary energy-region by region in an ill-defined way involving optimized fit to Jezebel criticality (too many other things impact criticality…) and Mosby. New Oct file uses a better methodology it seems but fits to 3 data sets (not 12) and it is not clear if weightings follow unc properly.
- Used 3 data sets; chi2 higher than INDEN

Capture

Rev. request on data ambiguities: (n,γ),<χ^2>



Evaluation	<χ^2> 0.0022-3MeV
B8 02/2018	3.0
INDEN β0a Feb 2022	✓ 1.61
LANL Oct 2022	6.8
LANL April 2022	6.8
LANL March 2022	11.5
LLNL β0c	8

INDEN GLSQ fit increases capture in B8 by up to 20% at 850 keV (suggested at CSWEG 2021, GLSQ fit in January 2022). INDEN is an improvement over ENDF/B-VIII.0 with reduced uncertainty. <χ^2> calculated by Zvview using exp. data and uncertainties

Capture reviews: Allan Carlson, SME reviewer

Capture

For INDEN, capture is obtained using GANDR for a generalized least squares fit of experimental data. It uses experimental data directly (Empire model calculation with large uncertainties is used as a model prior in GANDR fit for smoothing), not just based on a model calculation guided by data as in ENDF-B-VIII. Alpha (to give capture data using GMA fission data) and capture experimental data are used. The recent accurate capture data of Mosby is used in all three analyses. I think the INDEN method is better than using models as is done for both LANL (using modern reaction code CoH with input parameters carefully adjusted to reproduce experimental data.) and LLNL (calculated using YAHFC and was fitted by adjusting the gamma-ray strength function). I have always preferred analyses using experimental data directly. Doug Muir's code GANDR has had extensive work done to show its validity.
Below 100 keV LANL and INDEN look satisfactory. LLNL does not follow the data for almost all that entire energy range. It is consistently low relative to most of the data. Above 100 keV, again it falls low up to about a half MeV and above that it is just slightly above the measured data. It is not clear whether the LLNL results can justify the structure they have above a half MeV.

Overall, I would select the INDEN work on 239Pu fission and capture cross sections.

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Capture reviews: Don Smith – review requested

The Empire / GANDR approach used by the IAEA-NDS is well tested and mathematically well founded on the GLS approach. Slides 2-3 summarizes it well. A similar approach using different codes that follow the same math would also work, so the IAEA approach need not be unique. An example would be use of the GMA code which employs the same GLS approach. An advantage of intercomparison of results based on the same GLS concept but different codes is that it can potentially reveal subtle code differences that could influence outcomes, either in minor ways or possibly even more significant ones.

CAPTURE EVALUATION MADE USING CODE GANDR IS A TRUE GLS ANALYSIS. THE WORD "SMOOTHING" ALUDES TO THE FACT THAT MODEL-CALCULATED CROSS SECTIONS ARE INHERENTLY SMOOTH. Previous comment:
Consider the following sentence from this slide: "New capture evaluation is based on a GANDR generalized least squares fit of experimental data, not just on a model calculation guided by data as in ENDF-B/VIII.0 (Empire model calculation with large uncertainties is used as a model prior in GANDR fit for smoothing)". It should be checked with Roberto Capote whether this is completely equivalent to using Empire calculations (including covariances estimated from model-parameter uncertainties) to generate a prior and

introducing the experimental data in constructing the likelihood function. This would be the proper way of using GLS. The word that threw me a bit was "smoothing". Since Roberto and Andrej Trkov understand GLS very well (both for GANDR and GMA), I suspect that what they did is mathematically appropriate. It clearly differs from the approach taken in the recent evaluation from the LANL T2 group that I reviewed recently.
Don Smith says: NOTE IN REV01: ROBERTO CAPOTE HAS CLARIFIED THIS POINT. THE NEW CAPTURE EVALUATION MADE USING CODE GANDR IS A TRUE GLS ANALYSIS. THE WORD "SMOOTHING" ALUDES TO THE FACT THAT MODEL-CALCULATED CROSS SECTIONS ARE INHERENTLY SMOOTH.

Capture reviews: Don Smith – review requested (T2)

This cross section presents a situation where there are considerable available experimental data, including a new, comprehensive set of high-quality results from Mosby that were not considered in the ENDF/B-VIII.0 evaluation. Some of the available data sets agree reasonably well with others, while in other cases there are discrepancies with the main body of experimental information. Furthermore, there are some new developments in theoretical modeling to take into consideration. The authors of the current work take these factors into consideration, but it appears that is has been done in an ad hoc manner that is odds with the Bayesian approach and GLS, and thus he results are rather difficult to defend beyond the observation that they yield results that appear to be desirable. Furthermore, additional qualitative "tweaks" that are not too well defined in the document are applied to take into consideration some integral data. This is done without elaborating on well the spectrum to which these integral data correspond is known. So, it is suggested that the authors restrain from being influenced by the integral data in this particular differential cross-section evaluation for the ENDF/B library. Consideration of such integral data is probably best reserved for generating applications-tuned, adjusted libraries. Therefore, it is recommended that the authors consider investigating other approaches to evaluating 239Pu radiative capture that can be more readily justified on the basic statistical principles. One such approach would be to begin by producing a prior cross section with covariances based entirely on modeling. Choices of model parameters and their estimated uncertainties (uncorrelated) would be introduced, but in so doing an honest effort would need to be made to base these choices on experience as far removed as possible from consideration of available experimental data explicitly for 239Pu radiative capture reaction. Yes, that's easier said than done, but from the Bayesian perspective that is the proper approach. Then, all the available experimental data for 239Pu radiative capture should be

collected, examined, curated, and employed to produce experimental mean values and a corresponding covariance matrix. A straightforward GLS analysis would then be carried out in model-parameter space, with the parameters adjusted by GLS according to the influence of experimental data, or in cross-section space, whereby prior model-based cross sections and covariance would be calculated from the model and effectively averaged with the experimental information by GLS. This better-justified approach should yield evaluated mean values that probably will not differ greatly from the existing ones generated by the authors' work so far, and it would generate a posterior solution covariance matrix that appears to be lacking in the earlier work by the authors. It would be easier to justify the outcome because, to a considerable degree, this approach adheres to Bayesian procedures that are widely accepted at this time by the nuclear data evaluation community.

Capture reviews: Chadwick, SME reviewer

This reviewer suggests that a more traditional generalized-least square approach be used to evaluate capture, relying mostly on the measured data (with weightings related to the inverse square of assessed uncertainties). There are enough data sets (including Mosby) of sufficient quality to do this. Then one would have an evaluation that most faithfully represents our best understanding of capture. Also, this approach would then also provide fundamental-data based covariances.