

# CIELO: Status of Cross Section Progress

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*LANL*

Topics:

Oxygen: R matrix calculations; planned (n,a) LANSCE exp

Hydrogen scattering: Summary from Gerry Hale and Mark Paris

235U: Preliminary PFNS spectrum from Ch-nu @ LANSCE

239Pu; Data files created; PFNS; PFGS; TKE

## Abstract

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Progress is described for nuclear cross section evaluations, calculations, and experimental measurements at Los Alamos, on  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{16}\text{O}$  and  $^1\text{H}$ , for the CIELO project at NEA/WPEC. This includes first data from the Chi-nu project, providing insights into the energy spectrum of fission neutrons.

## Overview comments on CIELO progress

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Vast breadth of progress has been made on assessments – though new experiments, models, evaluations, MCNP simulations, of CIELO nuclei reactions

We're at the stage of “unbridled thinking” - “CIELO/A files”.

We'll be moving towards “disciplined implementation” towards some best solutions, with judicious choices perform well in integral calculations “CIELO/B files”

Examples of files that have reached a level of maturity...

- 235U g6 (and g6 mbc!) from IAEA, ORNL, & CEA file; 238U: ib44 from IAEA & Geel; 239Pu “version C” from LANL with SG34, ....16O, 56 files...

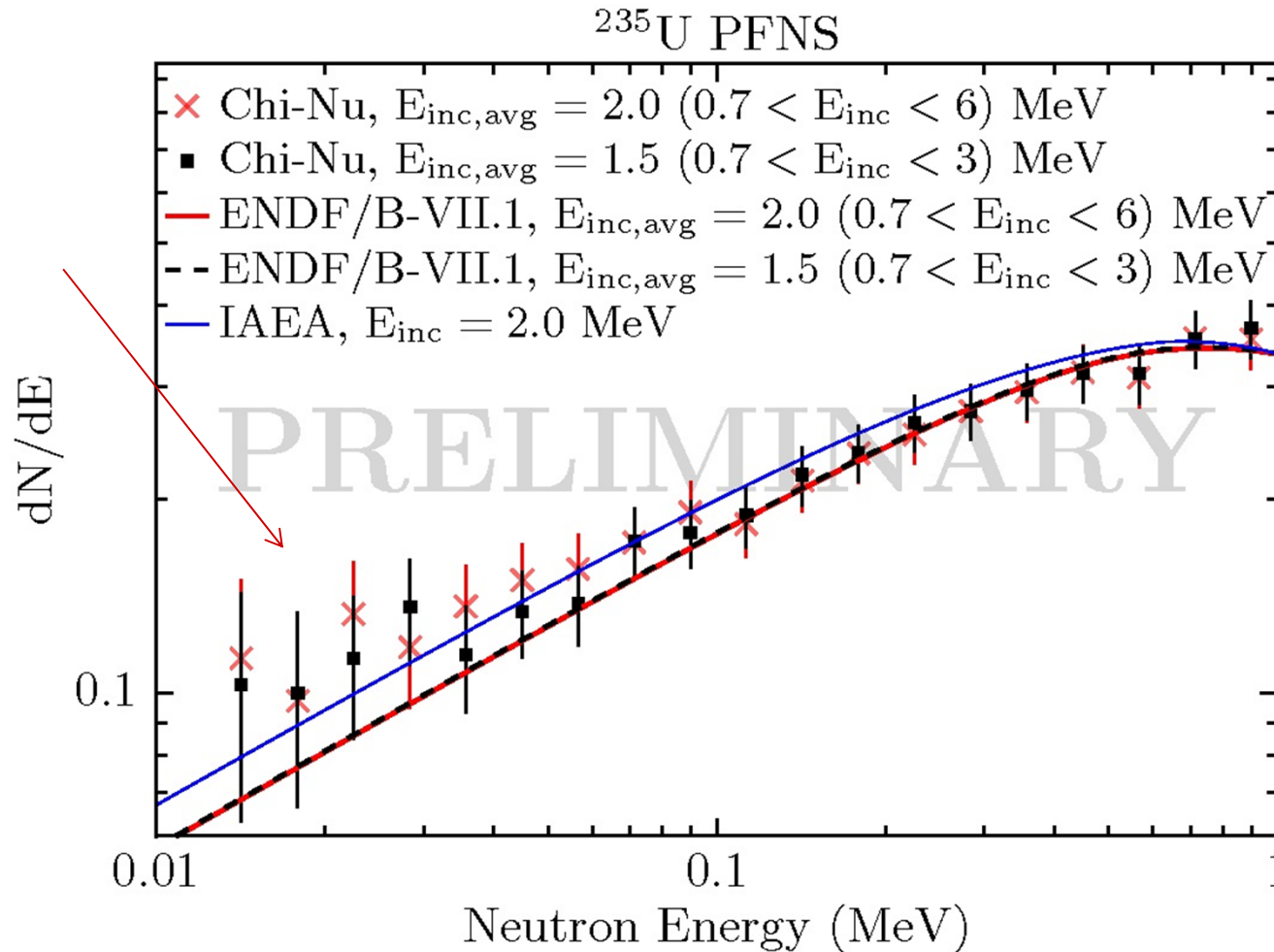
# $^{235}\text{U}$ : LANL PFNS Experimental Work in Fast Range (0.5-6 MeV) Suggests ENDF PFNS is Accurate

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- ◆ Lestone data was release last year for  $^{235}\text{U}$  as well as  $^{239}\text{Pu}$  PFNS (Published in ND2013 proceedings)
  - ◆ Einc average  $\sim 1.5$  MeV
  - ◆ E-emission  $> 1.5$  MeV
- ◆ New preliminary data from LANSCE/Chi-nu
  - ◆ Einc average – various “monoenergetic” and average energy cuts possible, including 1.5 and 2 MeV
  - ◆ E-emission  $< 1$  MeV in first phase of Chi-nu

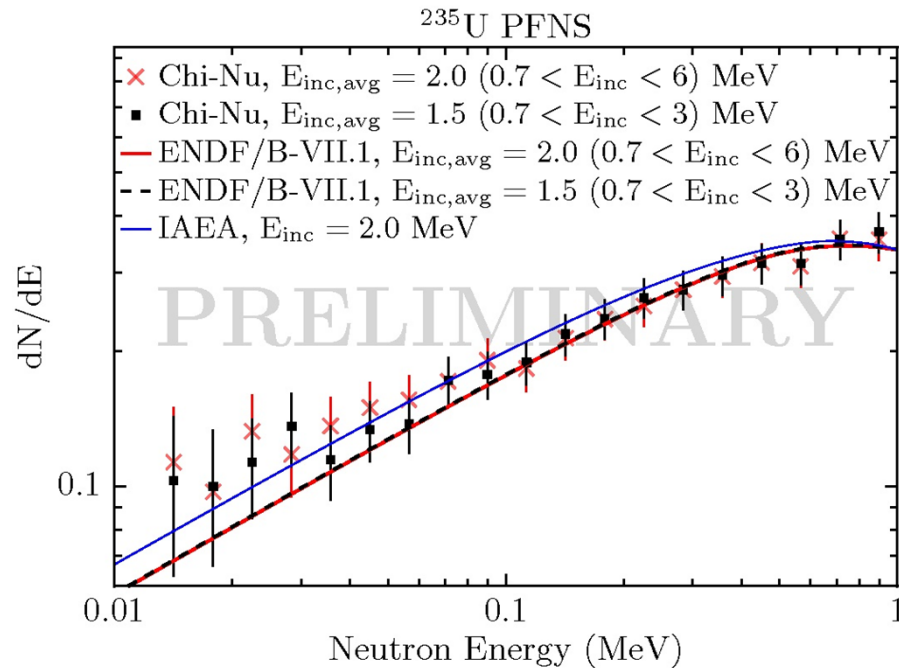
# $^{235}\text{U}$ : LANL PFNS Experimental Work in Fast Range (0.5-6 MeV) Suggests ENDF PFNS is Accurate

Below 0.1 MeV, backgrounds very high (6:1 ratio) and data less reliable



# $^{235}\text{U}$ : 2 LANL Experiments cover the whole emission energy range – Chi-nu (LANSCE) and NUEX (Lestone-Shores)

Eout < 1 MeV



Eout > 1 MeV

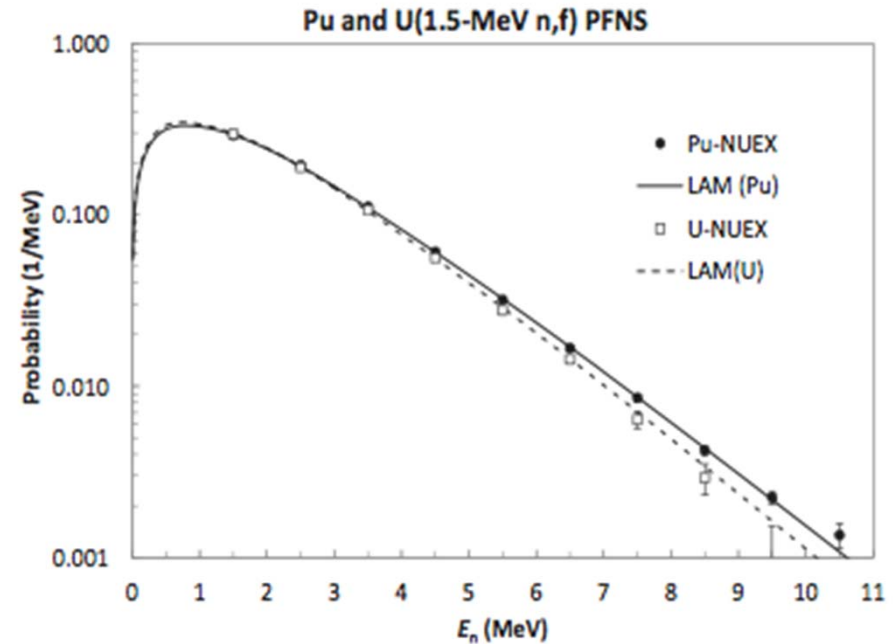


FIG. 3. The emission probabilities listed in Tables III and IV, and the corresponding 1.5-MeV n +  $^{239}\text{Pu}$  and  $^{235}\text{U}$  Los Alamos fission model fission-neutron energy spectra (curves).

## $^{239}\text{Pu}$ : Some Particular Challenges

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- ◆ Build on the excellent WPEC subgroup 34 work from CEA & ORNL
- ◆ Capture discrepancies. *We're waiting for final DANCE data; preliminary results obtained*
- ◆ New PFNS results coming (IAEA CRP etc), Chi-nu
- ◆ Inelastic scattering discrepancies between evaluations
- ◆ Use of new IAEA Standards, including fission (TPC)
- ◆ Other new data that will impact the evaluation – new PFGS data from DANCE; New FPY data from TUNL (impact esp at 14 MeV)

# Pu-239 Status. Version-0 performs like SG34 at low energies, ENDF/BII.1 at higher energies as expected (See Kahler talk)

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## ■ Contents of the Pu239 file CIELO/B -

- Based on ENDF/B-VII.1 cross sections
- SG34 resolved resonance parameters
- Prompt nu-bar in JEFF-3.2, up to 650 eV
- Total nu-bar re-calculated
- Base file uses ENDF/B-VII.1  $\chi < 5$  MeV; Romano tweak at thermal: Neudecker  $> 5$  MeV [Until we see Chi-nu 239Pu data, we are hesitant to deviate from ENDF in fast range]
- Variants: Other PFNS calculations from Neudecker et al.
- Huge section of delayed gamma-ray spectra removed

## ■ Some issues planned to be resolved in this and next years

- Unresolved resonance range, consider use of ISSF = 1 option
- Revise inelastic scattering, in collaboration with CEA/DAM, IAEA, and JAEA
- New gamma-ray production cross section, use of FILE6, and resolve inconsistent fission gamma-ray production
- Upgrade capture cross sections which considers new DANCE data

■ Slide 8

# Improvements in the new LANL evaluation –

## Neudecker work

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### □ Experiment:

- Recently published data of Chatillon et al. and Lestone et al. included (+ Granier corrections)
- Improved uncertainty estimate of exp. data (including Chi-Nu studies)

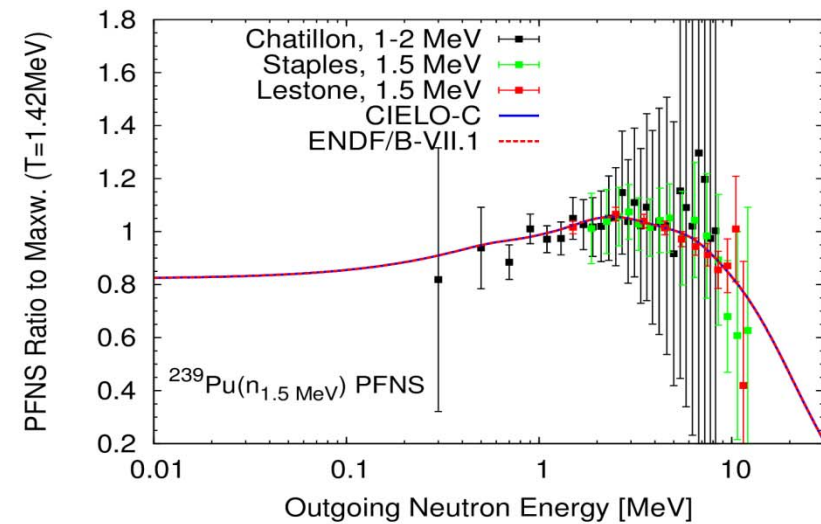
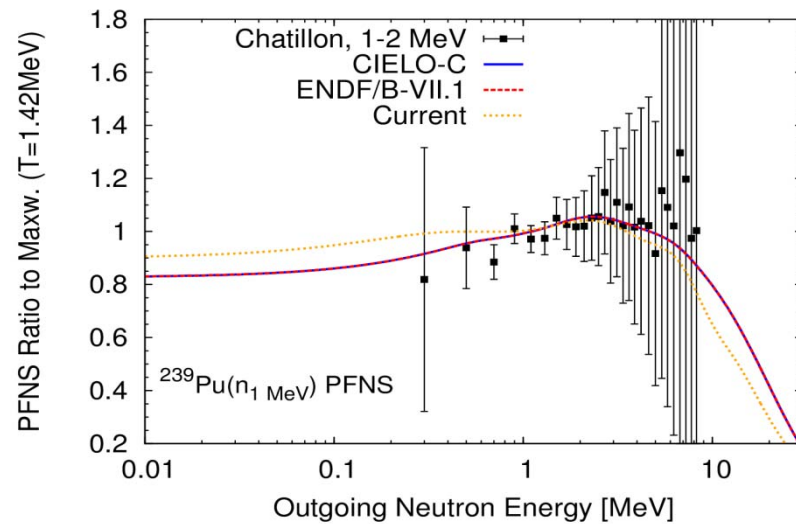
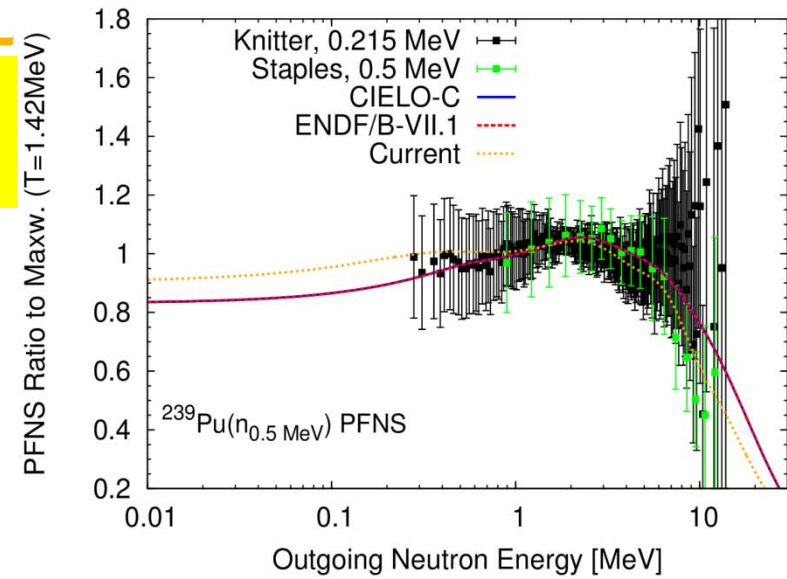
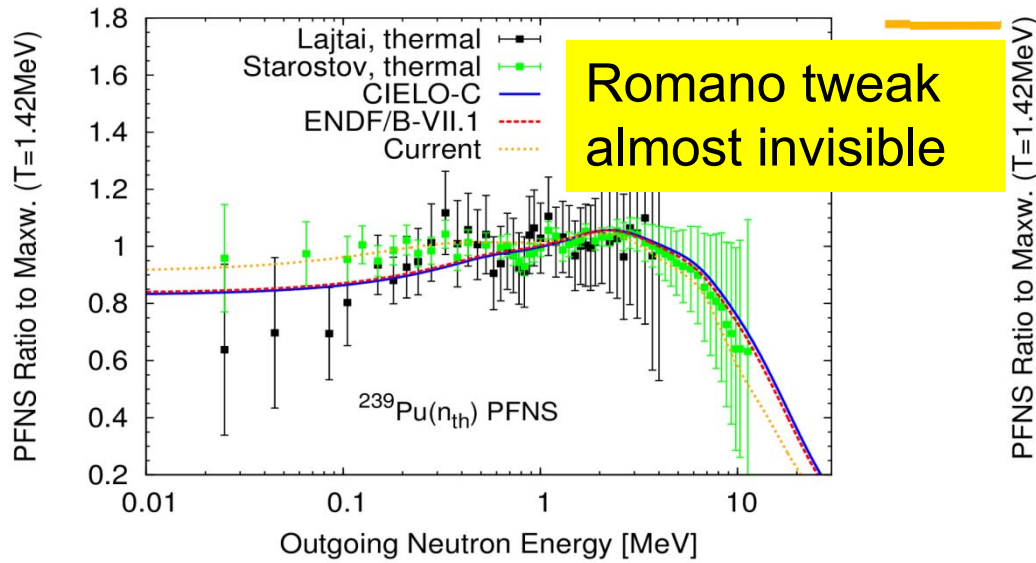
### □ Modeling:

- Einc-dependent parametrization of  $\langle TKE \rangle$  and  $\langle Er \rangle$  by Lestone et al.  
& Madland was used (constant for ENDF/B-VII.1)
- Pre-equilibrium component of the PFNS considered via CoH
- Only neutrons coming from the fission process are counted

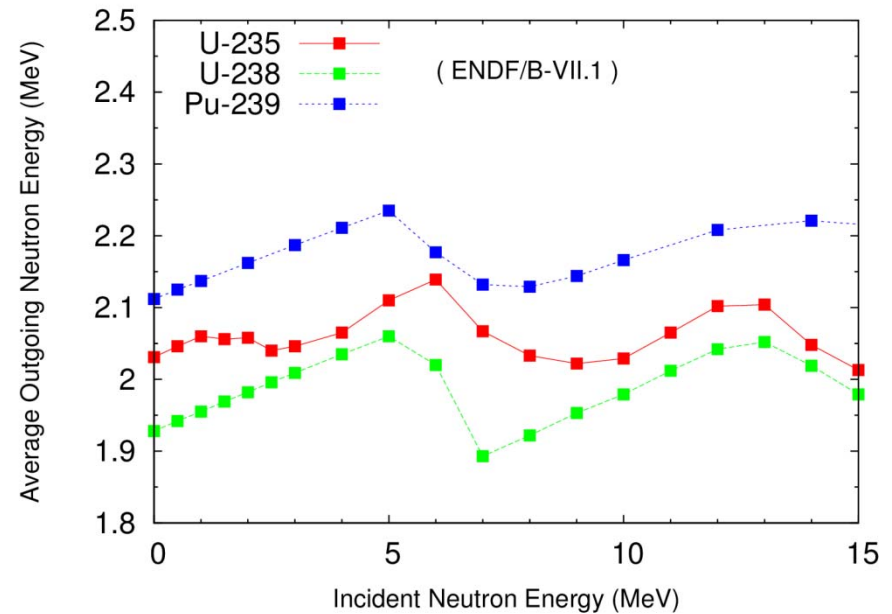
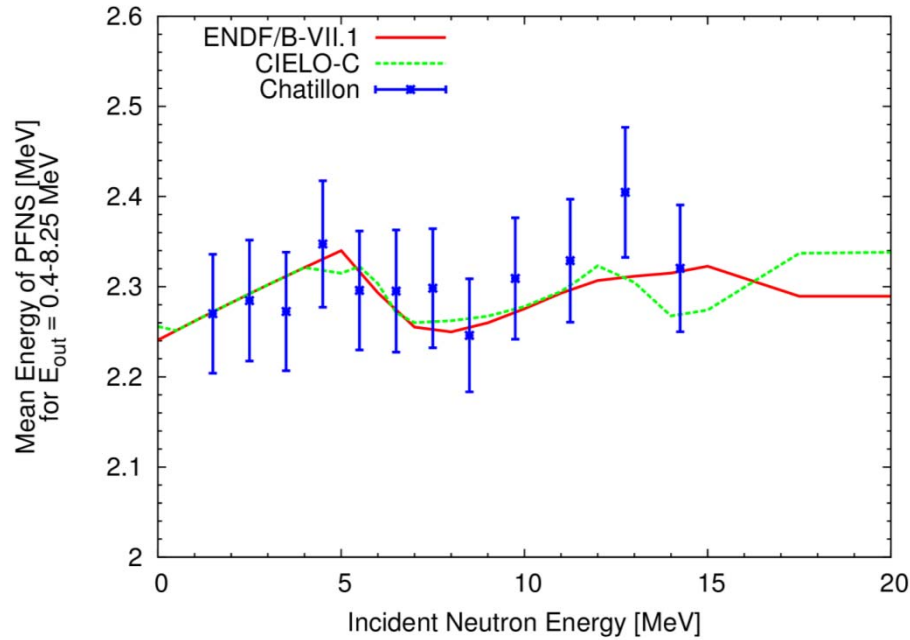
### □ Evaluated output:

- Given for Einc= thermal – 30 MeV
- Evaluated covariances are given for all Einc and also between different Einc

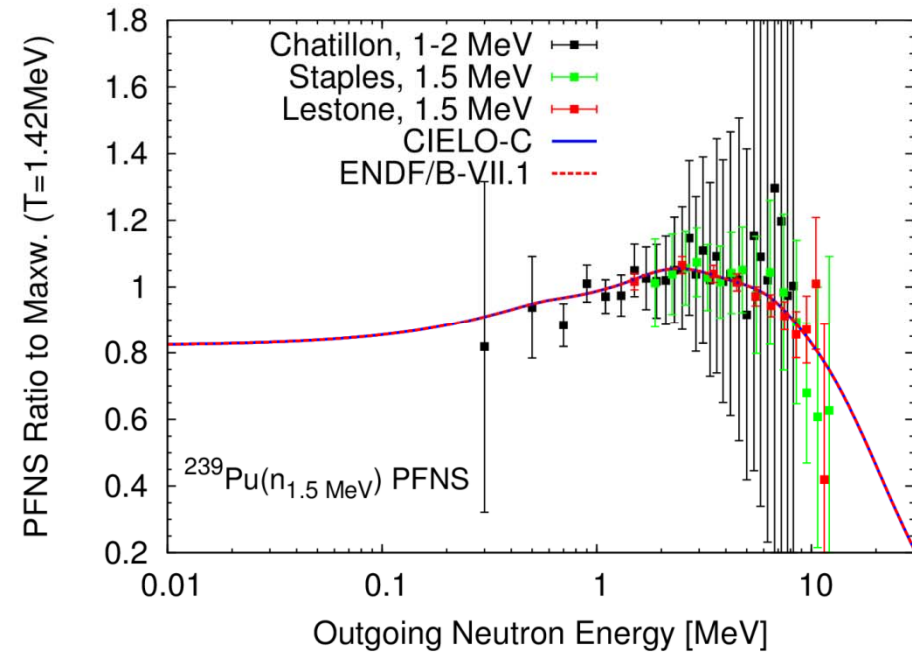
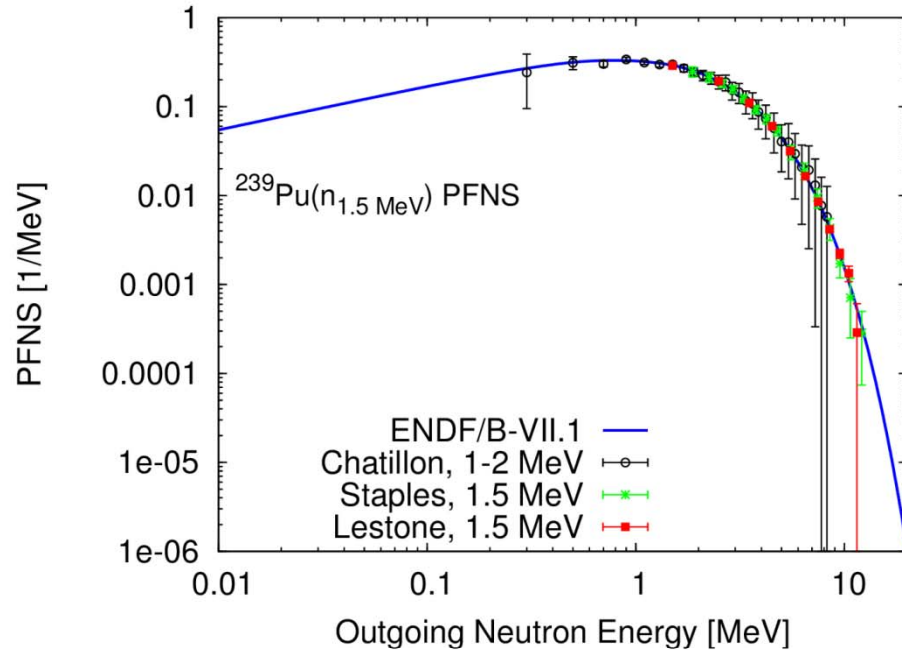
# 239Pu PFNS at all given Einc, Compared to Neudecker's Current Evaluation



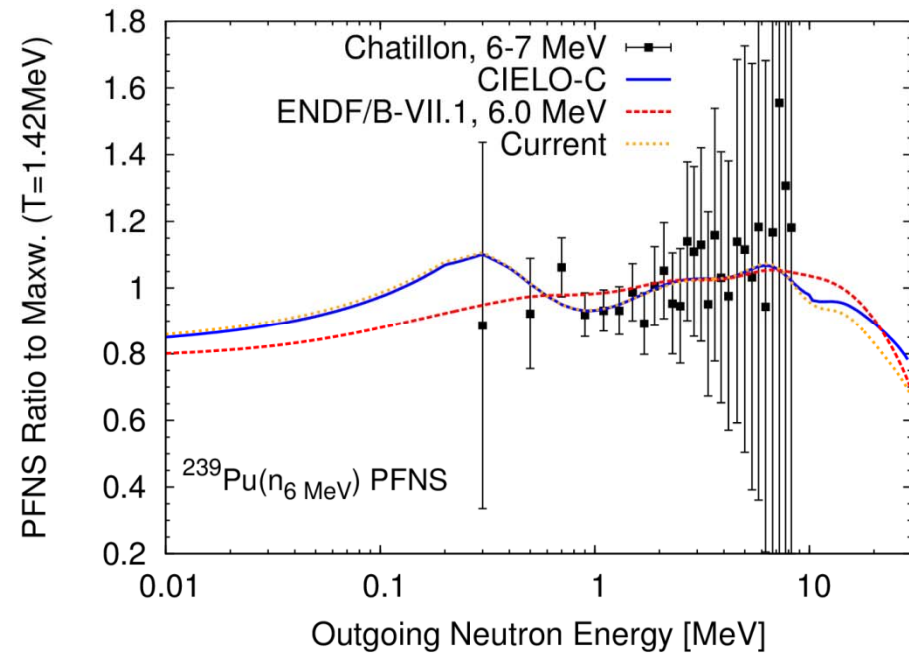
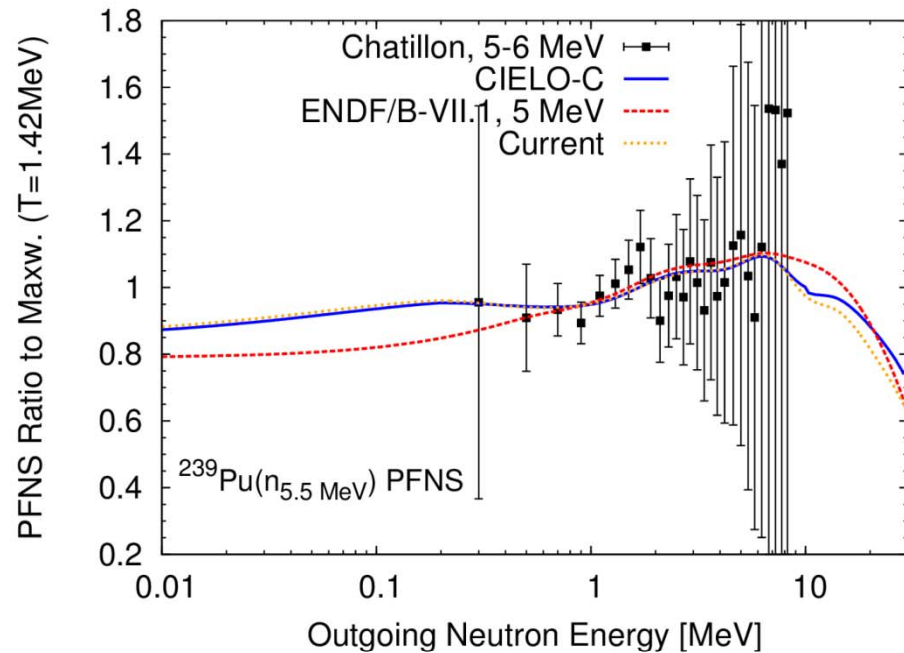
# PFNS Average Energy – CIELO file for testing (ENDF <5 MeV except for a tweak at thermal by Romano, and Neudecker > 5 MeV)



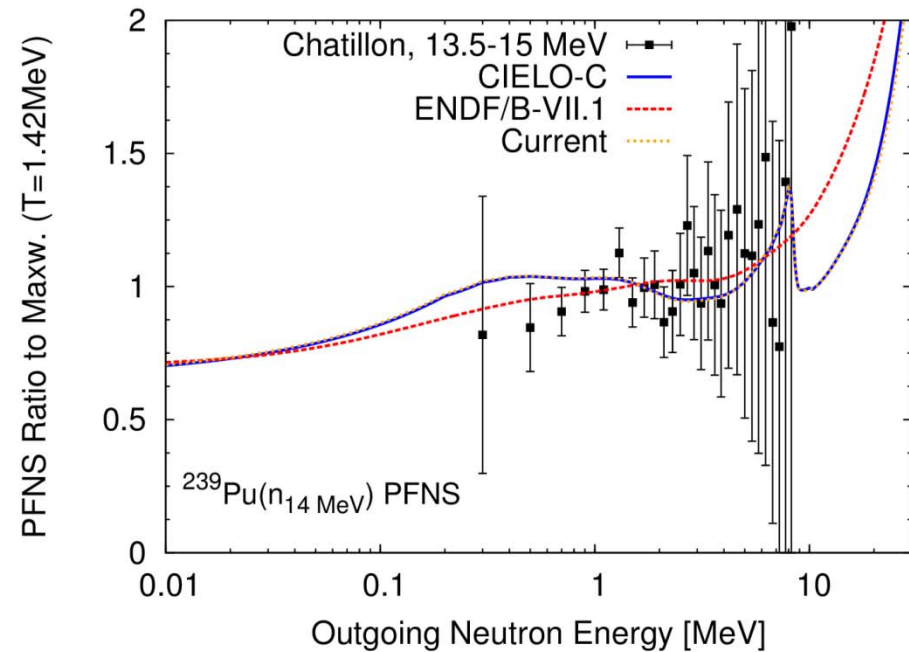
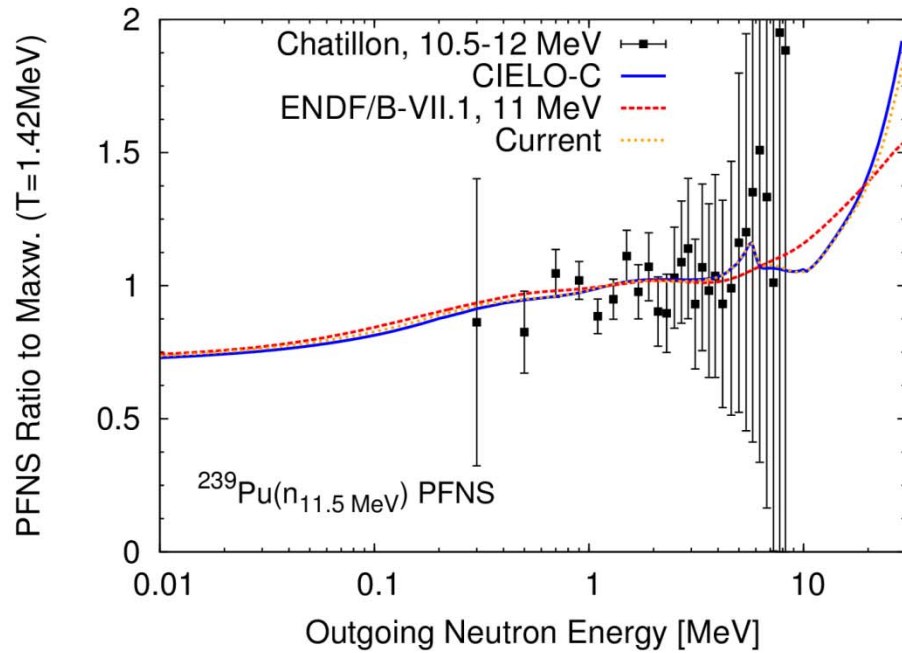
# **$^{239}\text{Pu}$ PFNS at $E_{\text{inc}} = 1.5 \text{ MeV}$**



# **$^{239}\text{Pu}$ PFNS at $E_{\text{inc}} = 5.5\text{-}6\text{ MeV}$ (opening of second chance fission)**



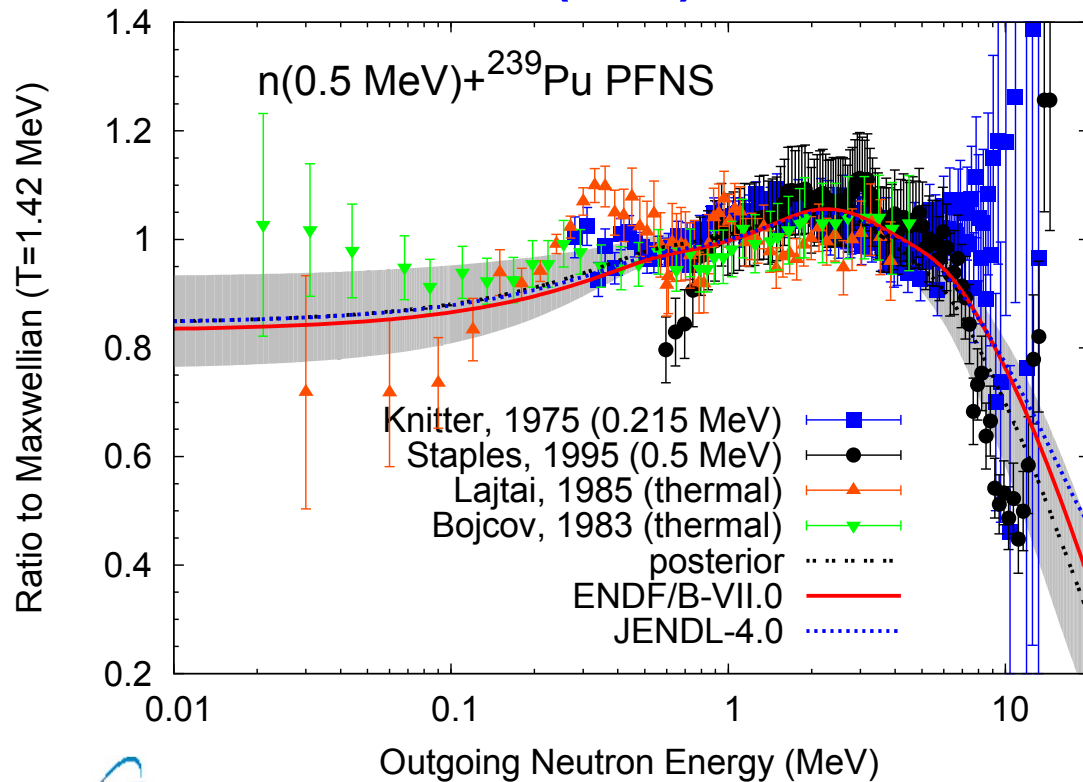
# **$^{239}\text{Pu}$ PFNS at $E_{\text{inc}} = 11.5 \text{ MeV}$ and $E_{\text{inc}} = 14 \text{ MeV}$**



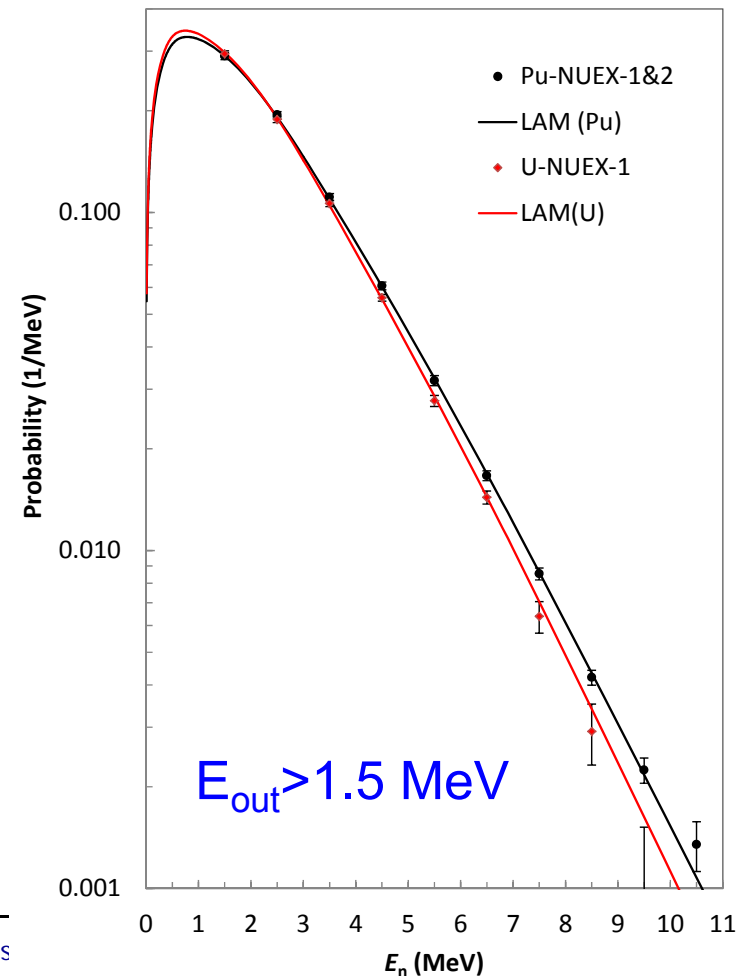
# Determining the Prompt Fission Neutron Spectrum (Chi): One of Our Highest Priorities & an IAEA CRP. Chi-nu PFNS delayed till next year (235U measured recently)

Large uncertainties below 1 MeV and above 5 MeV impact criticality calculations and (n,2n) transmutations

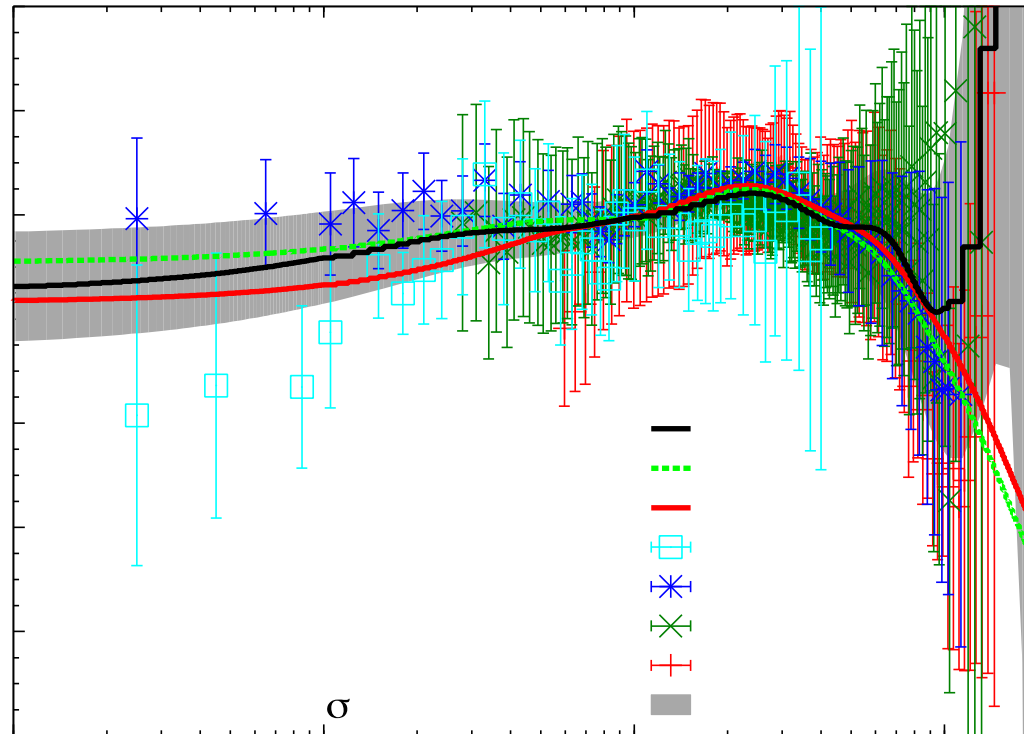
Lestone's talk: *accurate* underground NUEX data released by Los Alamos:



Pu-NUEX-1&2 and U-NUEX-1 (1.5-MeV n,f) PFNS

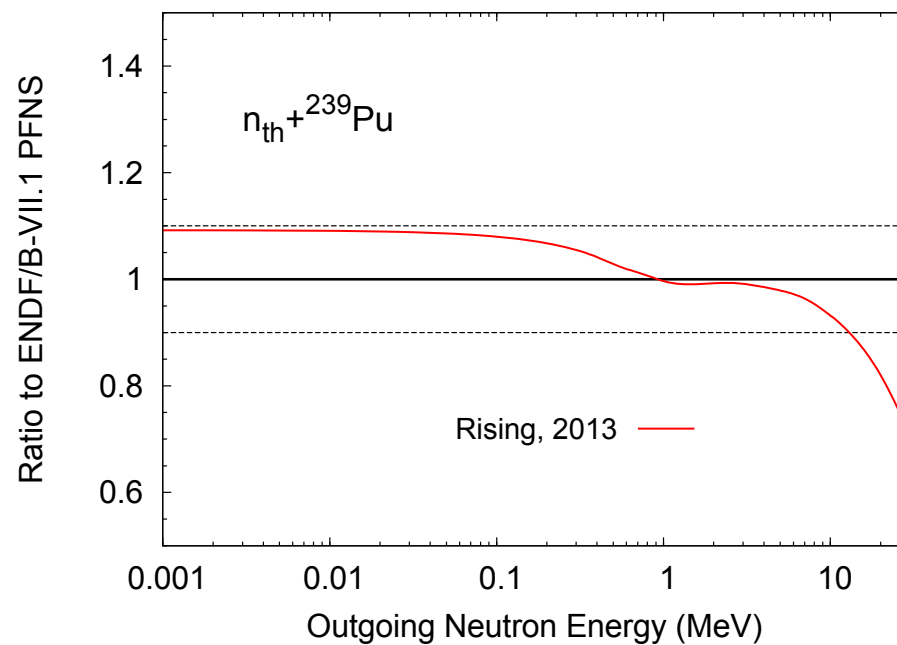


# Ongoing work on PFNS by Talou, Reisner, Neudecker (red = cielo.0 ; green = cielo.1)



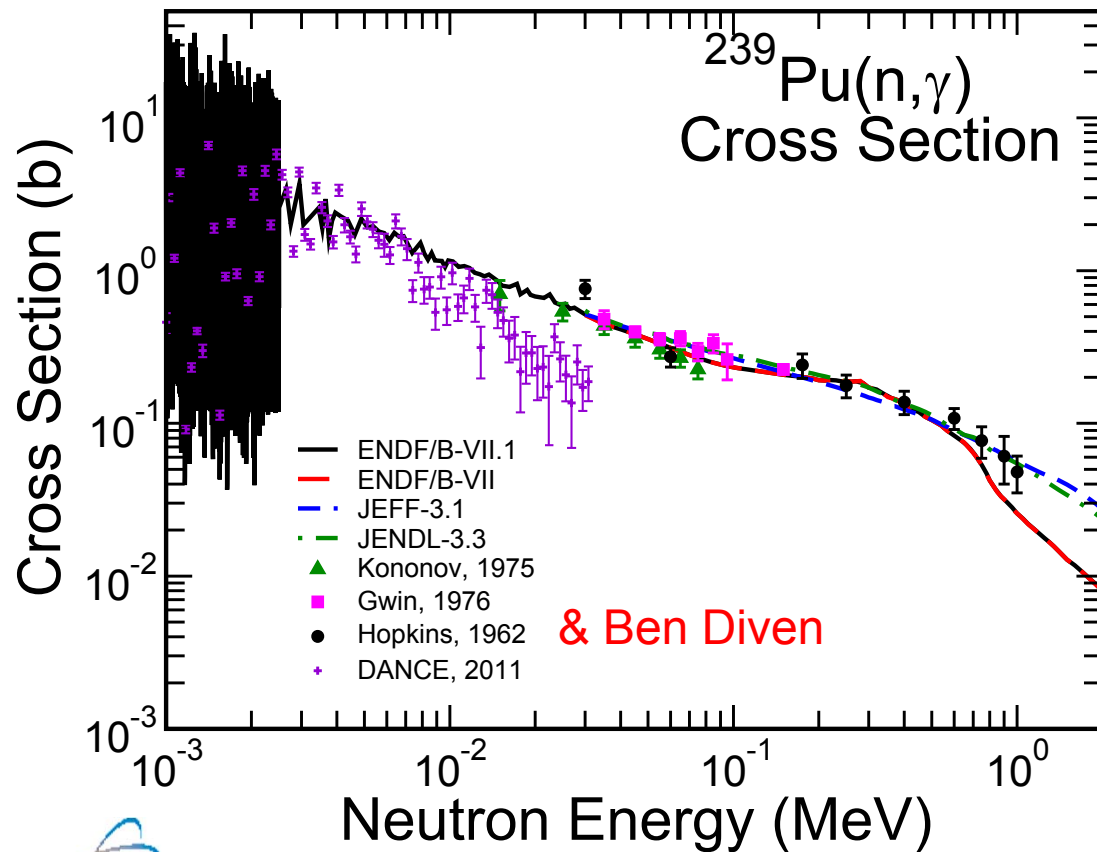
Black = snapshot of ongoing work. Will be updated to include Lestone, Chatillon, etc

# Ongoing work on PFNS – Reisner result for thermal, in file cielo.1 for testing



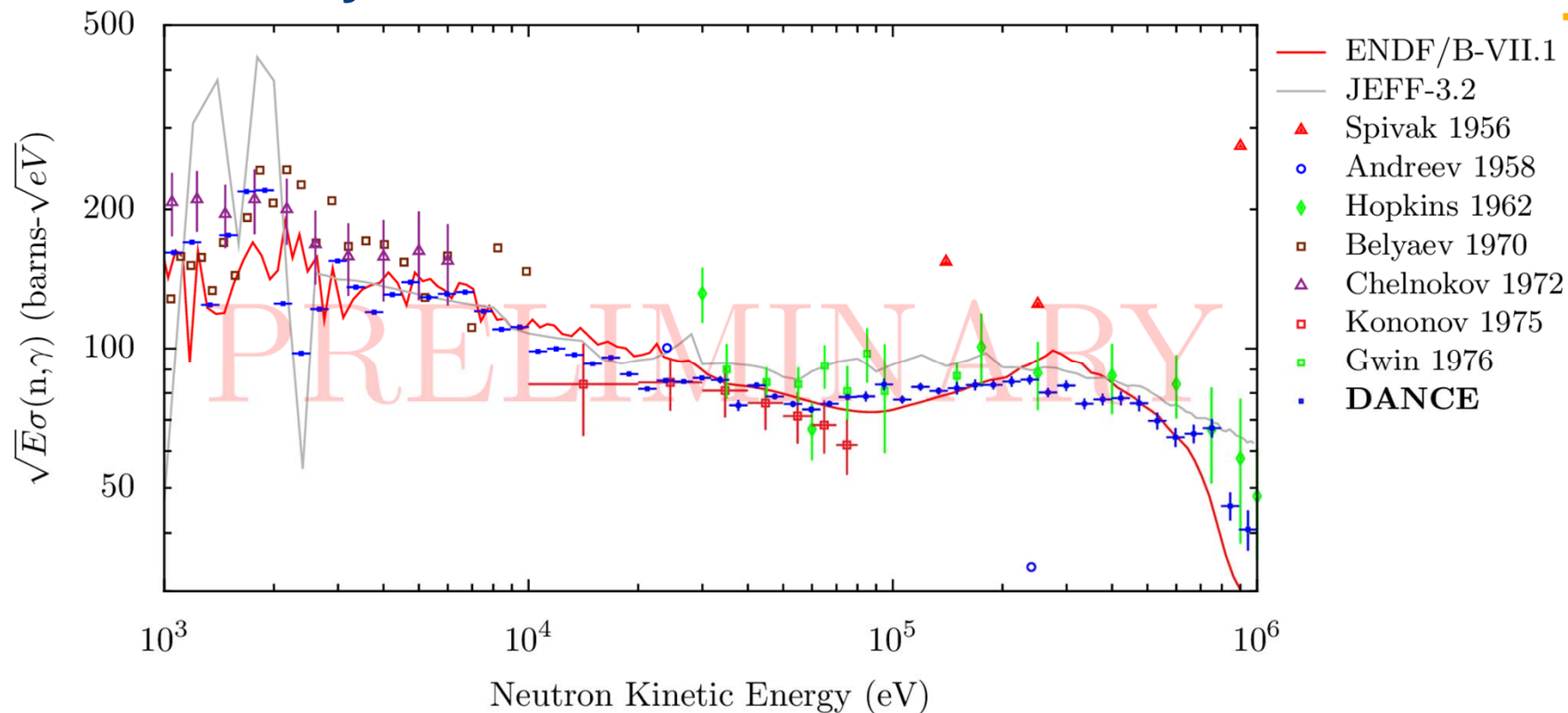
# Plutonium Capture: Improvements Are Needed

Existing uncertainties >15%



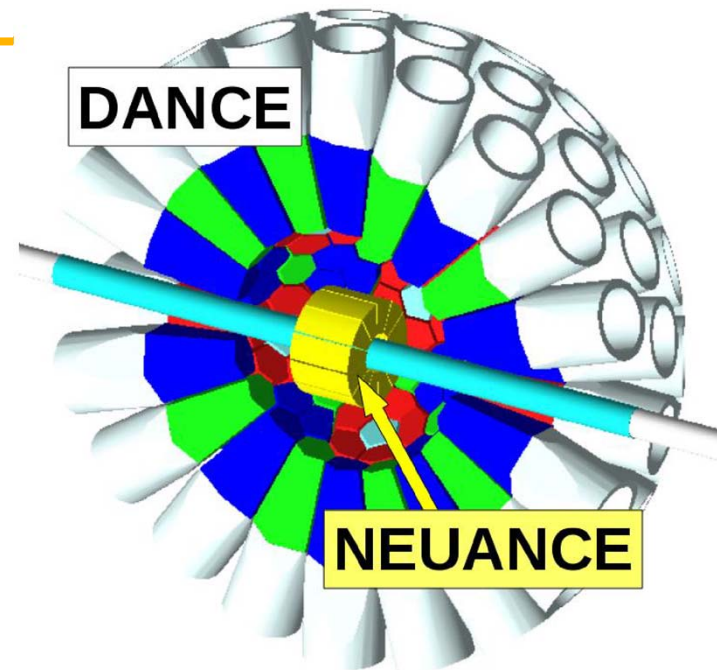
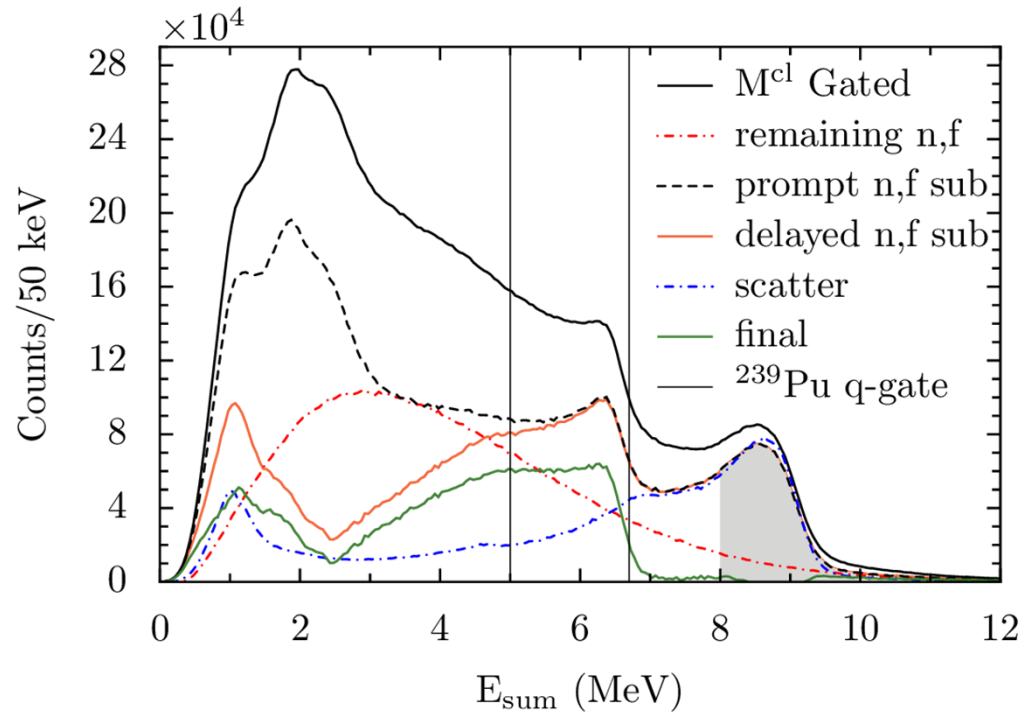
- SG33 & PROFIL (PHENIX)  $^{239}\text{Pu}(n,g)$  integral testing suggests B-VII is ~ 10% low over this fast reactor spectrum. Also, Ishikawa's ADJ work suggests JENDL should be raised 5-10%
- DANCE measurements now being analyzed

# Preliminary Results for $^{239}\text{Pu}$ from DANCE



- Investigating structures in keV region
- Plan: complete analysis by end of this FY
- What will be the impact on criticality calculations?

## How could we improve?



- Fission and scattered neutron background strong above 10 keV (left)
- Neutron detector inside DANCE (right) could reject much of this
- Prototype detector run in January – optimizations are needed

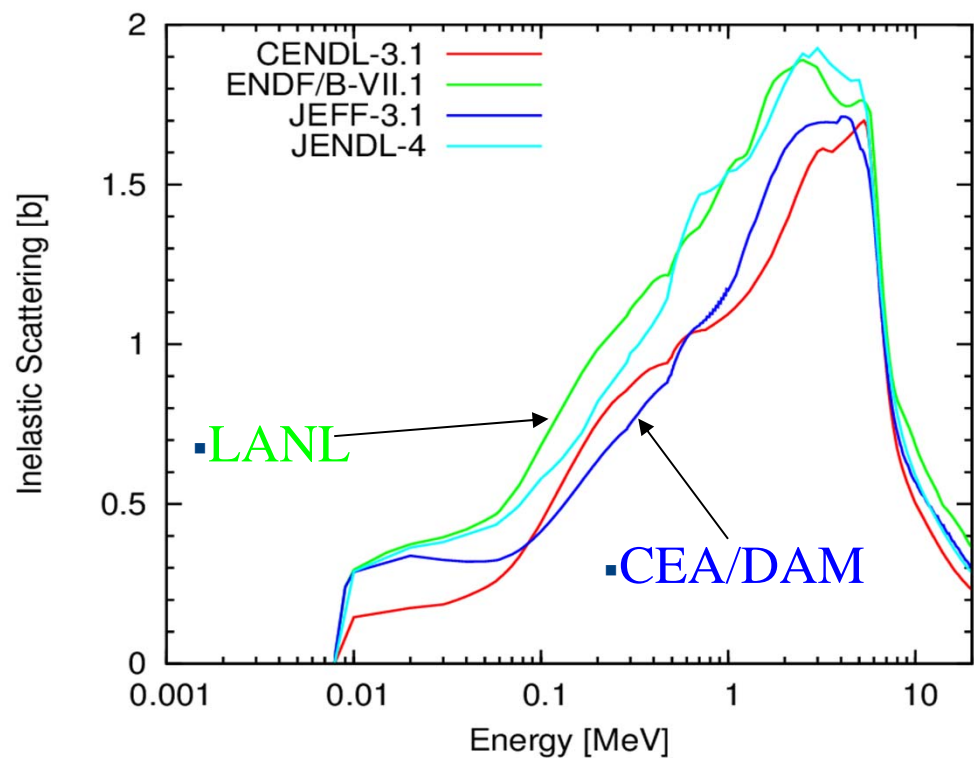
# Inelastic Scattering Discrepancy

- **IAEA Technical Meeting on Model Calculation for Major Actinides**
  - Summary report published: INDC(NDS)-0597, R. Capote, et al.

▪ These two files equally work for Jezebel keff prediction.

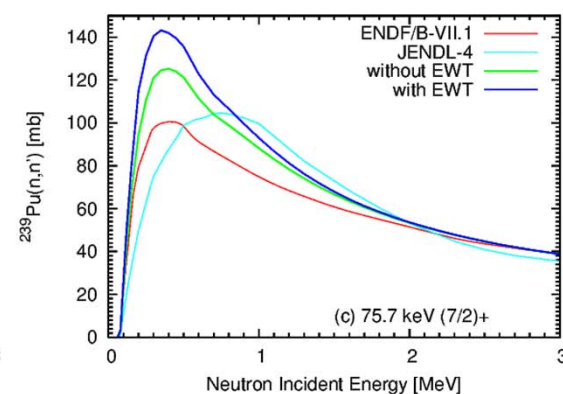
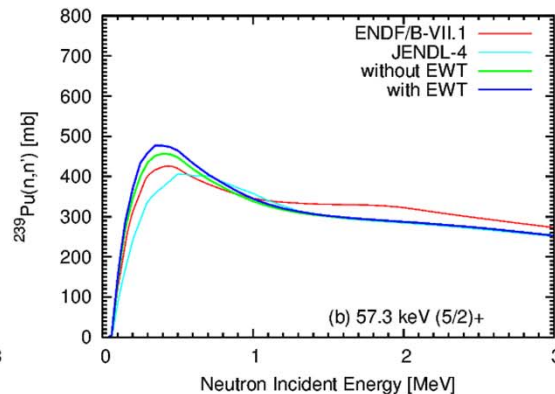
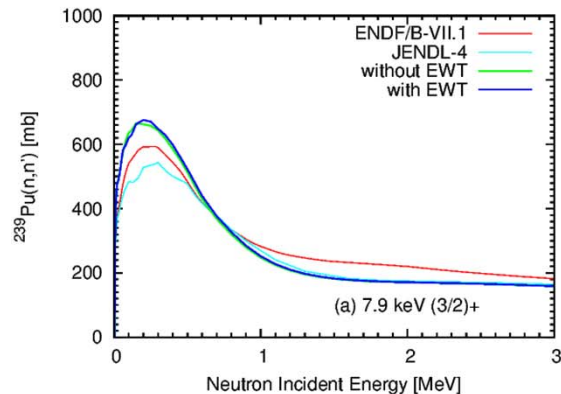
▪ Probably, the difference in the inelastic scattering comes from the optical potential parameters adopted in each library

- CEA total cross section is higher than ENDF in the 30keV - 500keV range
- total and absorption cross sections anti-correlated



# Pu-239 Inelastic Scattering - Kawano and collaborators

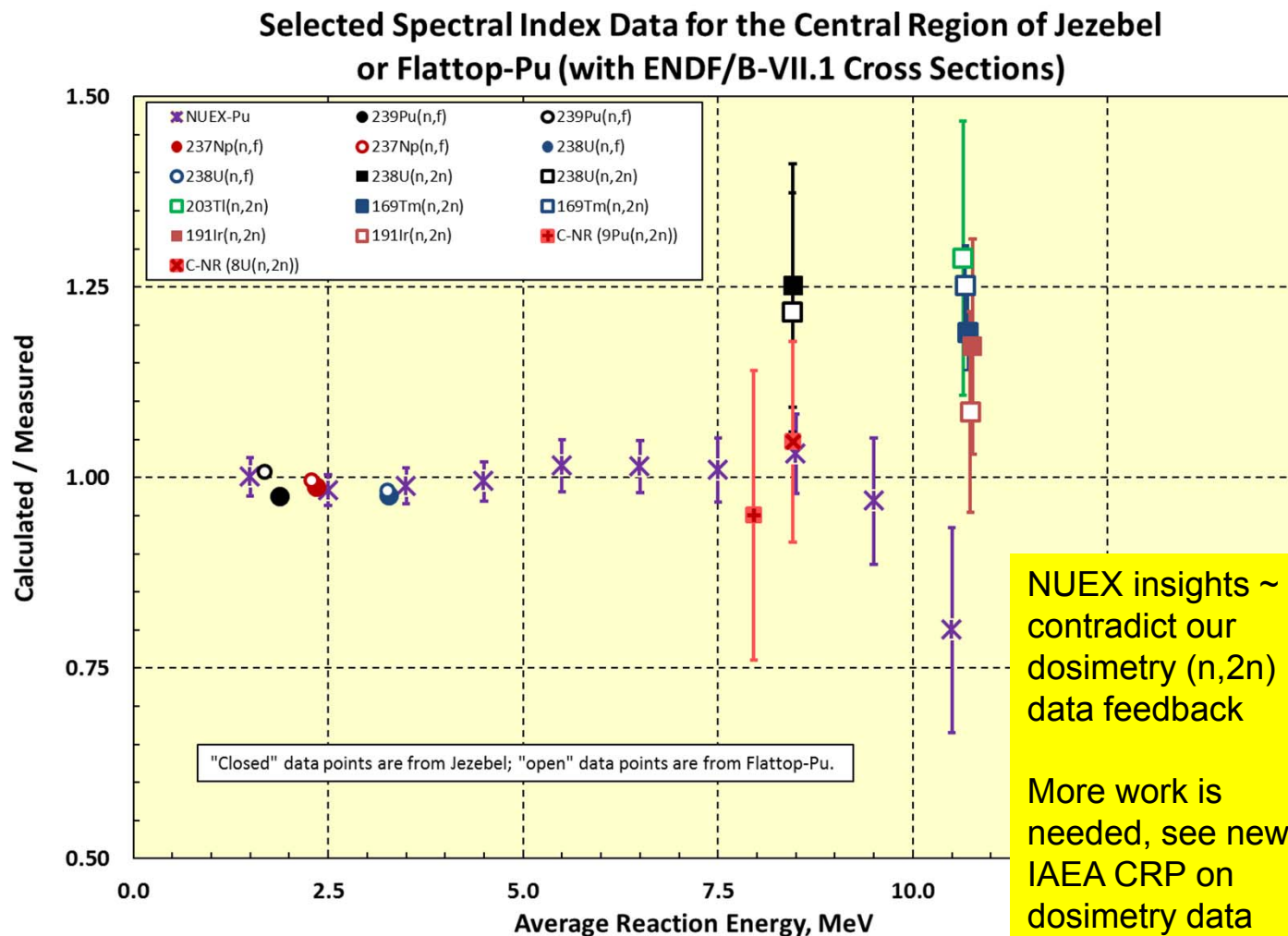
- **Correct treatment of compound cross section**
  - Full Engelbrecht-Weidenmueller (EW) transformation performed
  - Fission channel has not yet optimized
    - higher than evaluations
  - Difference between the EW and Hauser-Feshbach-Moldauer cases seems to be small



# Reaction Rates in Fast Critical Assemblies Provide Integral Test of Prompt Fission Neutron Spectrum & (n,2n) Cross Sections - *Plutonium-239 PFNS Data*

239Pu

With NUEX  
data added  
(Lestone)



NUEX insights ~ contradict our dosimetry (n,2n) data feedback

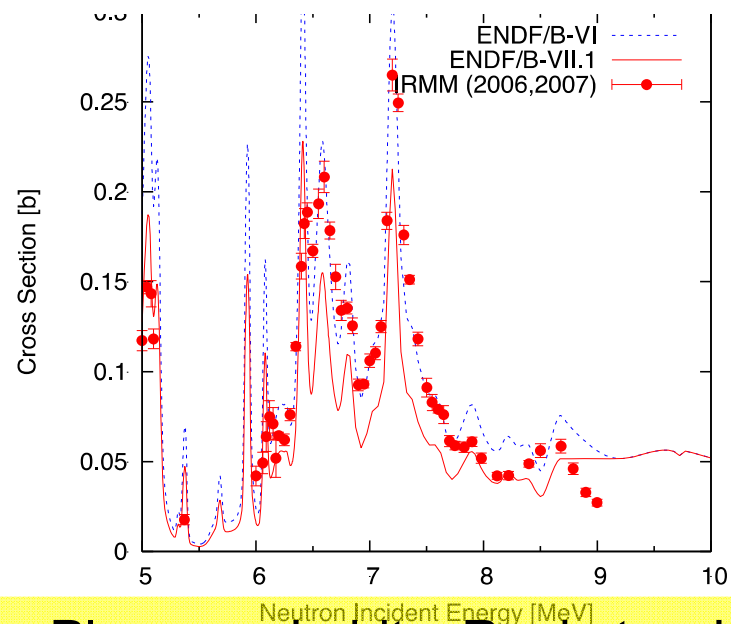
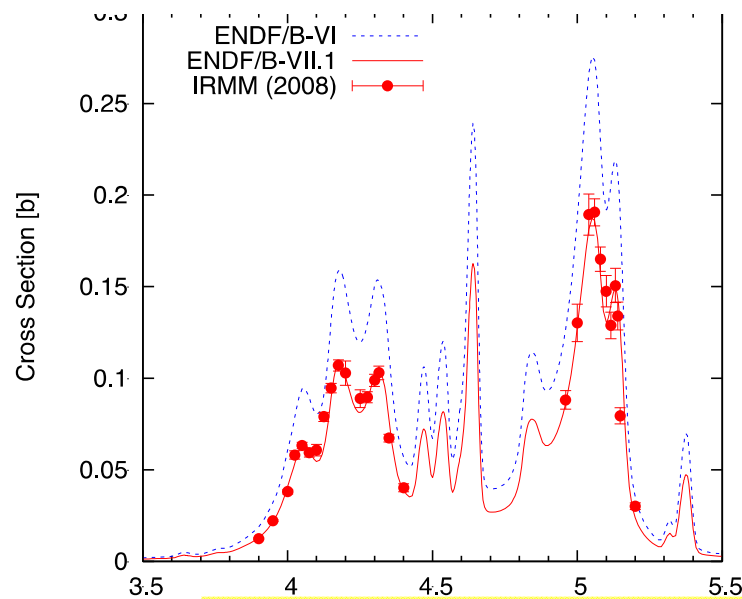
More work is needed, see new IAEA CRP on dosimetry data validation

Cecil Lubitz:

*“After several “preliminary” months on CIELO it’s clear that we have bitten off a big chunk. Get ready to chew.”*

# $^{16}\text{O}$ . Work is Needed to Reconcile R-Matrix Theory & Data & Maintain Criticality and Transmission Performance

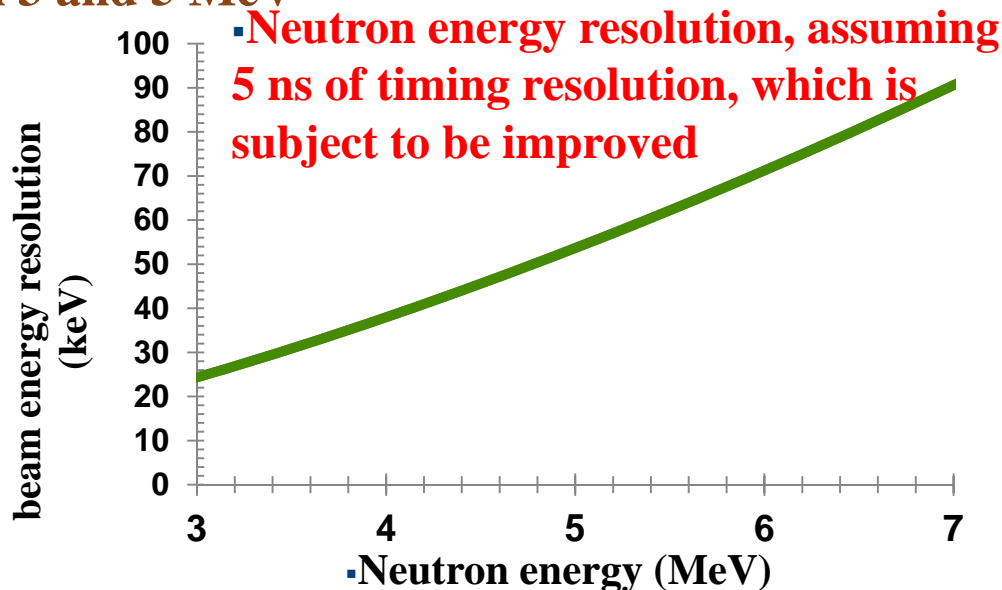
(R-matrix theory + total cross section data seems to suggest a higher (n,a) than measurements. Geel is now revising their (n,a) data upwards too).



Progress being made by Plompen, Lubitz, Roubstov, Hale, Kunieda, Leal, Moxon, Kopeccky ... **LANL plans a measurement**

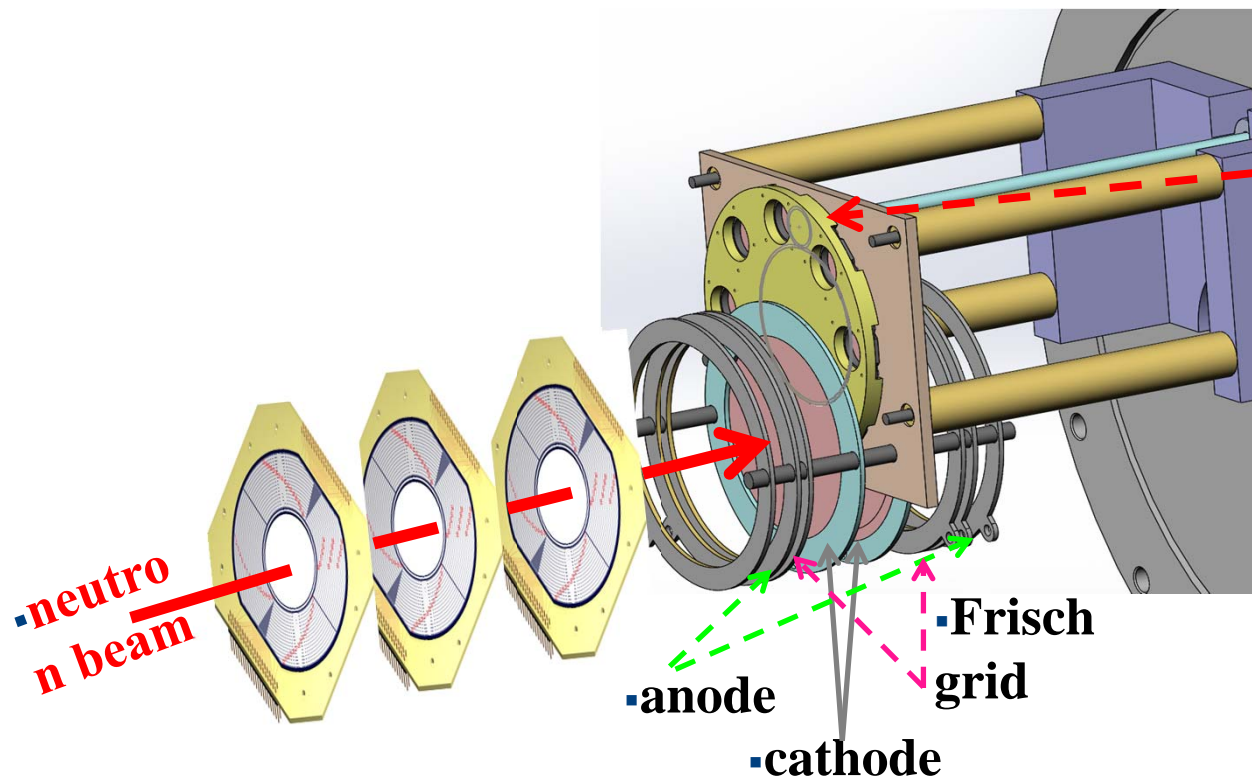
# LANL plans to measure new cross sections on $^{16}\text{O}(n,\alpha)$

- Use a newly developed instrument LENZ with a large solid angle and low alpha detection threshold
- Use a white neutron source at WNR/LANSCE in Fall 2015
- Relative measurement to  $^6\text{Li}(n,\alpha)$  reaction to reduce systematic uncertainty
- First goal is to measure cross sections at the energies between 3 and 5 MeV



▪ Picture of LENZ chamber

# LENZ : Twin Frisch-grid Ionization Chamber + Silicon Strip Detectors



- The multiple target system allows to have a oxygen and a Li reference target at the same time
- Solid oxygen target is made by anodizing highly-enriched water on tantalum backing

○ At forward angles, the silicon strip detector measures angles and charged particles energy deposit

○ Digitizers provide wavelet information for post processing of improvement of signal-to-noise ratio with no dead time

## Hale comments on new (n,tot) RPI data:

Comments about LANL n+<sup>16</sup>O Cielo evaluation:

The evaluation we submitted in June of last year is similar in many ways to ENDF/B VI.8. For that reason, since the total cross section was preserved in the evaluation that finally became ENDF/B VII.1, it is not surprising that the agreement with the new RPI measurement of the total cross section looks similar for VII.1 and the LANL Cielo file. Our latest evaluation is somewhat better in the "window", and somewhat worse at energies above about 4.5 MeV. Adding these total cross section data to the analysis would likely decrease the total cross section somewhat in the 2.5-3.5 MeV region, which because of the often-noted anti-correlation effect of unitarity in this region, would tend to raise the fitted (n,alpha) cross section at these energies. This would make the disagreement even worse with experiments that favor the lower normalization scale for the reaction cross section.

We are anxious to add these measurements (not the binned data) to our analysis to see what their effect might be, but we are gratified that the initial comparison does not seem to indicate any major problems with the evaluation. Hopefully, we will have additional (n,alpha) data coming from Los Alamos in the next year or so. In the meantime, we are working on extending the existing LANL file above 6 MeV, and including the Geel (n,alpha) data in our analysis, following Giorganis' recommendations about normalizations, etc.

3	<b>160</b>	
4		
5		
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7	General	
8		Intercompare evaluations, and identify goals for a new evaluation
9		
10		JENDL is a new work (though adopts ENDF n,a); ENDF (JEFF uses ENDF) is a hybrid of KAPL work < 3.2 MeV, LANL (Hale et al) > 3.2 MeV - assess value of
11		The 2005 ORNL work generated a resonance analysis for 16O, full R-matrix. Included angular distributions, n,alpha, and it has never been tested. Needed L
12		
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14		
15	Total, Elastic and inelastic scattering	
16		Compare existing evaluations and R-matrix analysis, and define path forward
17		
18		At low energies, assess whether evaluations of elastic scattering indeed need to be lowered by ~3%, as proposed by Plompen, Lubitz, Roubtsov etc
19		
20		covariances for muon: Need reliable anisotropic 16O scattering uncertainties. Palmiotti thinks Gerry's present uncertainties are too small on muon.
21		
22	Capture	ENDF adopted JENDL's capture cross section to include resonance contribution - establish consensus to use this
23		
24		
25	(n,a)	
26		Review different evaluations (all largely same as ENDF)
27		Review previous data, and agree on scales - eg Bair & Haas had renorm their original data down by ~20%; Are Johnson data the same as these?
28		
29		Review new data - Georginis (Geel), Khryachkov (IPPE) - contact physicists working on 13C(a,n) for astrophysics
30		The above new data approx confirm ENDF below 6 MeV but point to changes above
31		Intercompare R-matrix calcs (Hale, Kunieda, Leal)
32		Seek to understand why the above R-matrix evaluations, influenced by total cross sec data, suggest ~30% higher (n,a) than most measurements
33		Define an evaluation strategy... If theory contradicts these data, do we use data instead? Or do we conclude theory is right and measurements had a scale error
34		Assess whether evaluations (all now based on ENDF) above ~ 6 MeV need changing, if it is concluded new Geel data are more accurate than old Davis data
35		
36	Integral	Establish suite of integral validation tests, including k-eff, transmission, etc
37		2 benchmarks sensitive to oxygen data (+11 more benchmarks with water) are available in the SINBAD database
38		Broomstick experiment
39		Following WPEC SG? , With the existing (n,a) evaluations perform well, for the most part, on LEU solutions, Can the new eval perform well too
40		(n,a) impact at higher energies: Does this higher energy >6 MeV region impact any applications significantly (maybe medical applications)? Carlson notes M
41		check astrophysics constraints on 13C(a,n) reaction rate
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$^1\text{H}$

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Gerry Hale, Cecil Lubitz:

*Advancing the  $^1\text{H}$  analysis, for the next standards update, by adding new data*

*Focus below 20 meV, and extending to higher energies (150-200 MeV)*

## 1H & Other Standards: Hale's Summary and Outlook

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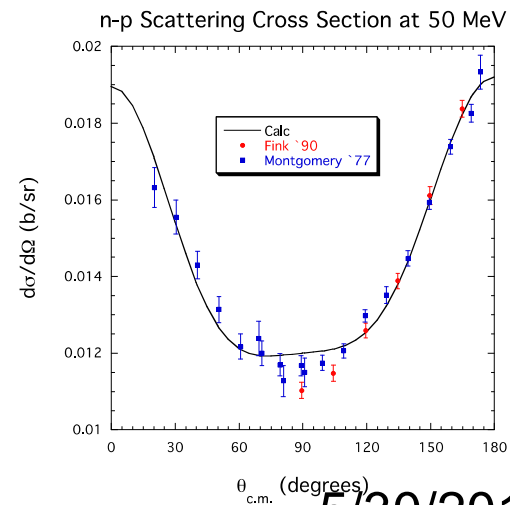
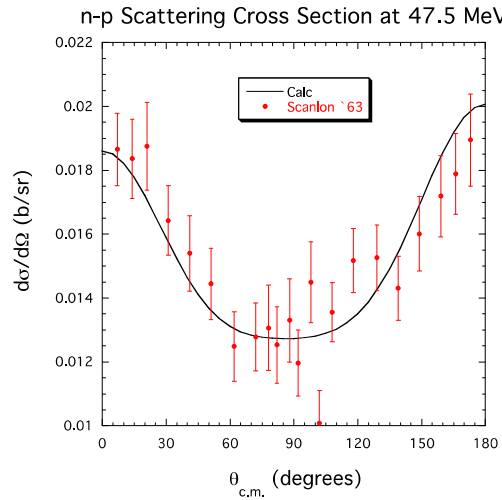
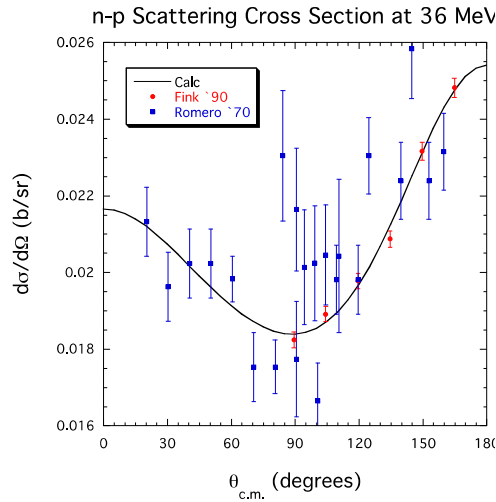
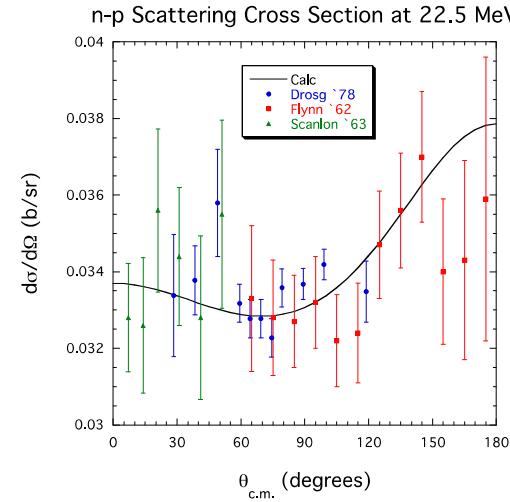
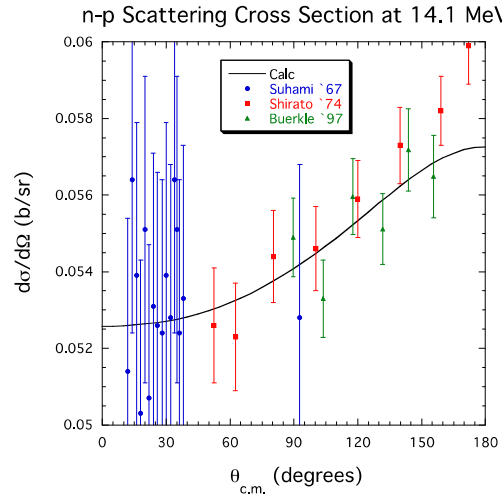
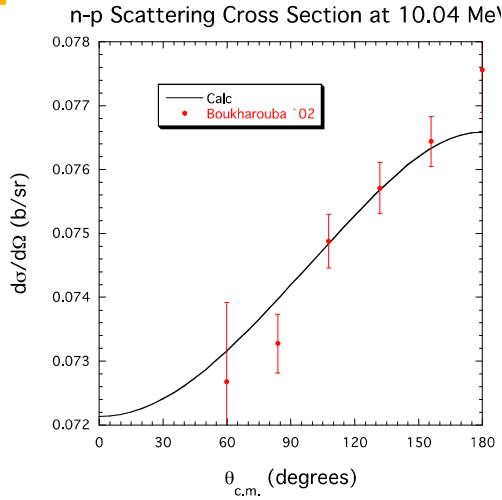
- **NN analysis progressing; more p-p elastic scattering data needed in the 30-50 MeV range. Low-energy parameters retain their earlier (correct) values. Need to extend analysis above 200 MeV.**
- **New data for n+<sup>6</sup>Li fit in well with the existing data set, and cause no problems with the R-matrix fitting.**
- **n+<sup>12,13</sup>C analyses in good shape below 2 MeV. Could produce a natural C standards file in this energy region now. More work is needed on both evaluations at higher energies, however.**
- **Problem with unrealistically small uncertainties on standards cross sections may be solved by using parameter confidence intervals.**

## **$^1\text{H}$ – Hale comments on the covariance data**

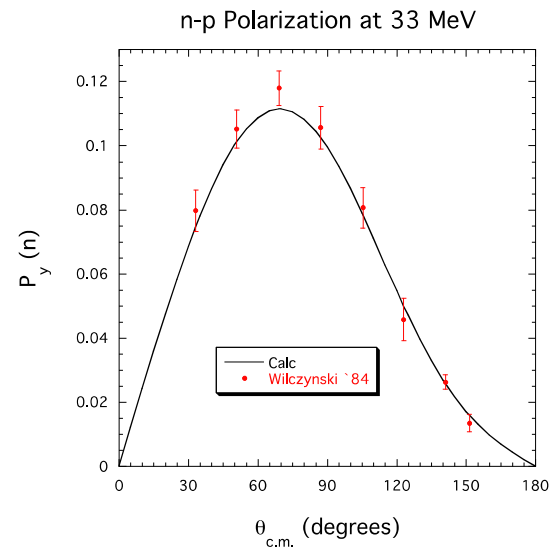
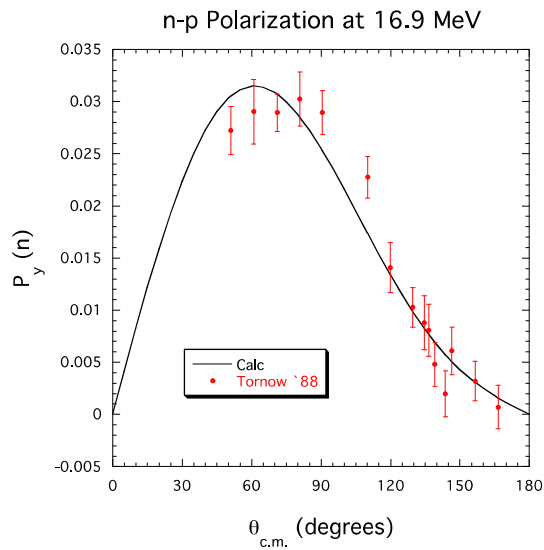
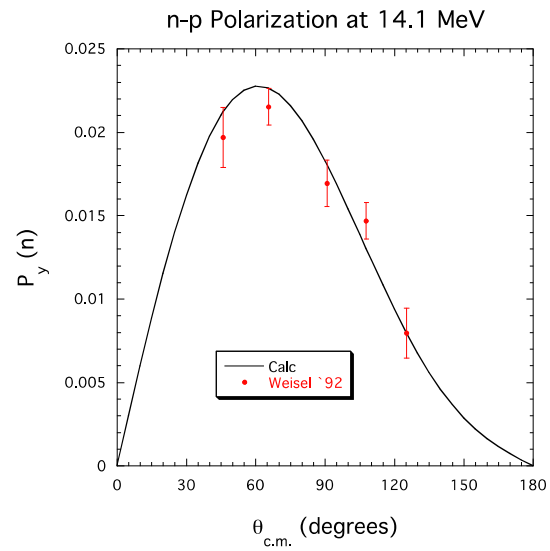
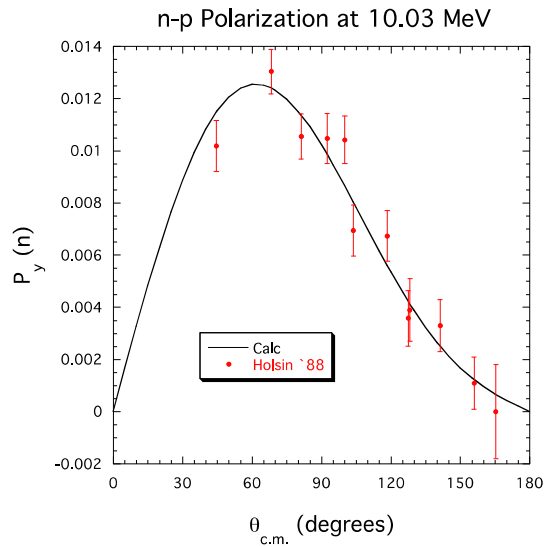
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*The uncertainties in the n-p scattering cross sections that were put into VII.1 (as described in my CW 2008 paper) are fairly realistic (maximum of 1% at around 10 MeV). The uncertainties on the capture cross section are probably too large, due to the kludge I had to make to compensate for Lubitz's insistence that the thermal value be a certain number. All of this should be better in the next release, since we will use confidence intervals in place of standard deviations (which has the effect of scaling up the standard deviation by a known amount)*

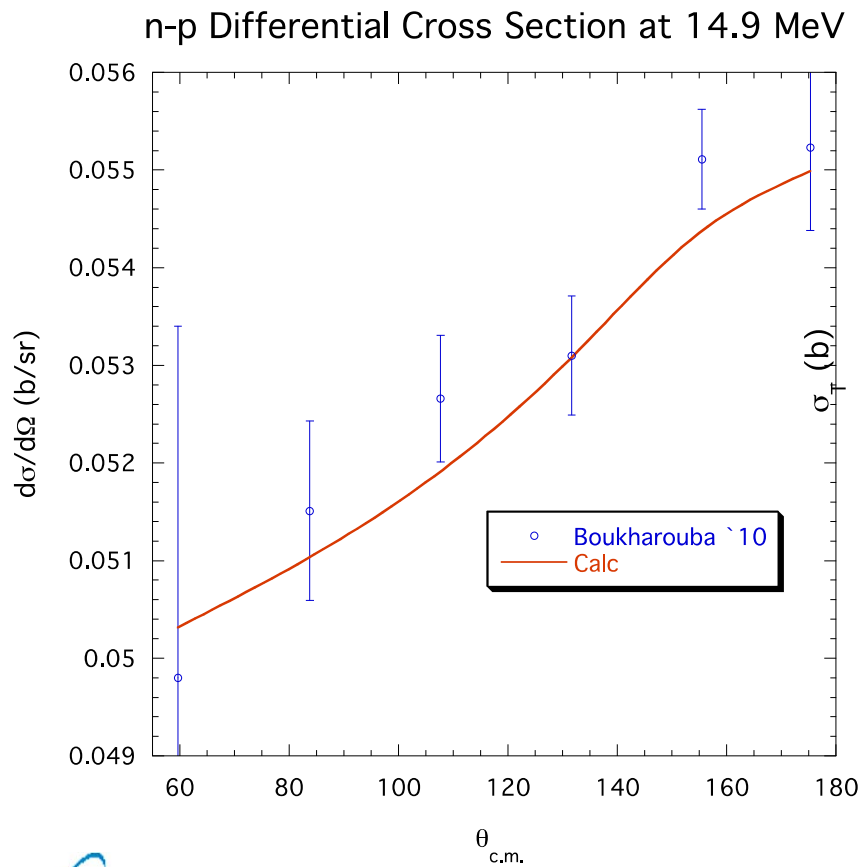
# n-p Differential Cross Sections



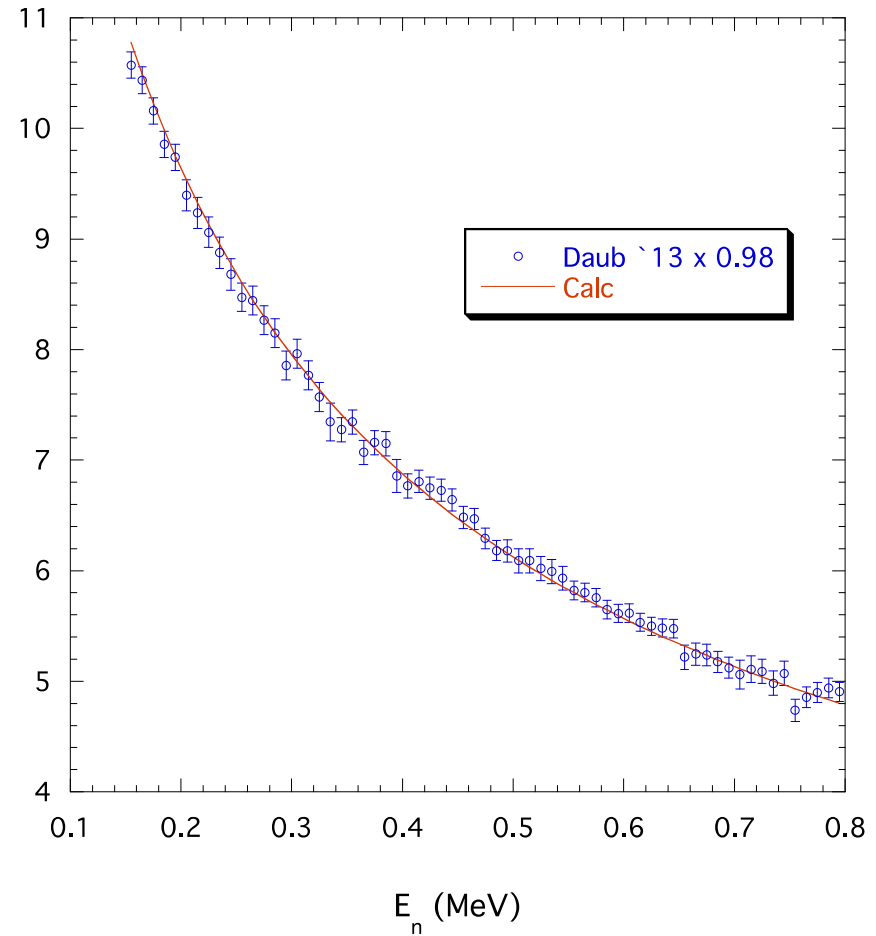
# n-p Polarizations



# $^{11}\text{H}$ recent data added to analysis



n-p Total Cross Section



## Summary ...

CIELO collaboration is making progress.  
Plan for next stage needs to be developed.



# BACKUP SLIDES

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## **Backup: In Case You Didn't Think We Have Lots of Work .....**

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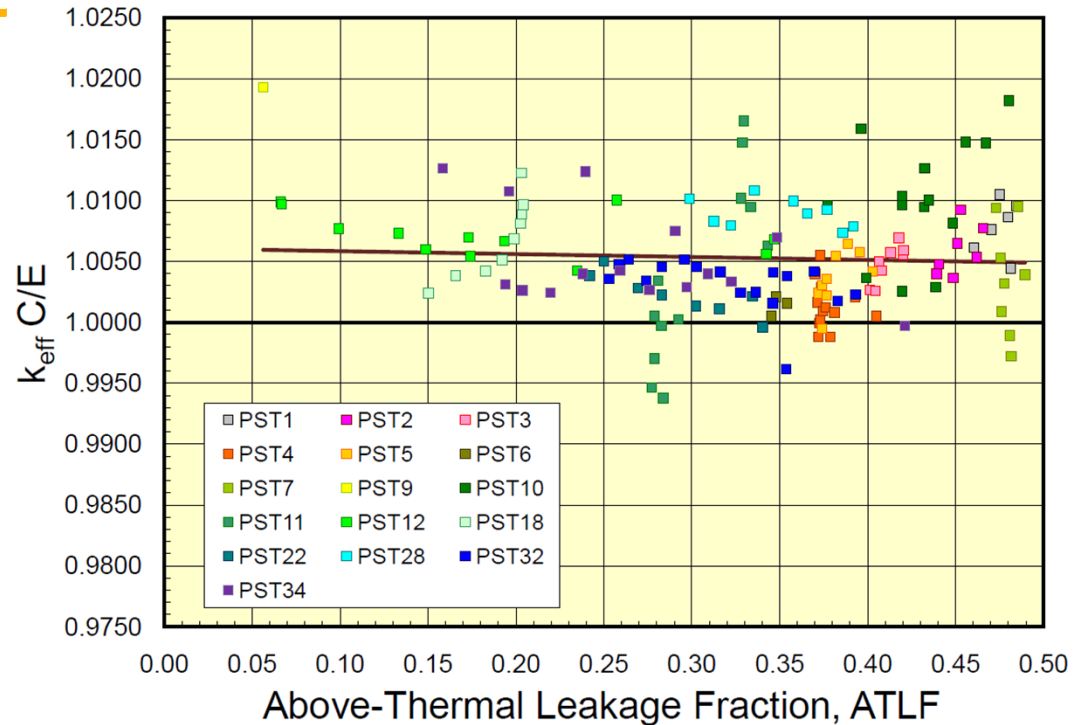
	A	B	C	D
1	CIELO: Summary of tasks to address:			
2				
3	<b>Actinides: 239Pu, 235U, and 238U - specific issues for each nuclide are noted</b>			
4				
5	Fast Region (keVs and above to 20 MeV) - fission listed separately			
6				
7	Review Overall Goals, as embodied in this document and in LAUR CIELO document			
8				
9	Inelastic and elastic scattering - below a few MeV (eg 7)			
10	Review existing discrepancies between evaluations			
11	Collect all available experimental data			
12	Review various theoretical approaches, as embodied in codes (including HF, Coupled Channels, KKM, ....)			
13	Discuss and review optical model options			
14	238U: dispersive coupled-channels OM developed at IAEA			
15	Seek consensus on best evaluated representation of data			
16	238U: 238U Elastic and inelastic scattering data from RPI. Quasi differential available (mainly inelastic) from RPI from from 0.5 MeV up to 20 MeV. - EN			
17	235U: New (n,xng) data to be published in PRC by Kerveno et al. (IPHC, Strasbourg (F)) could be useful to model inelastic scattering on first levels, see			
18	Understand implications from integral data testing on changes in inelastic scattering - especially k-eff and reaction rates (spectral indices for 85/5f etc)			
19	Assess covariances and implement in ENDF format			
20	Create ENDF formatted files			
21	Inelastic and elastic scattering - 7-20 MeV			
22	Review existing discrepancies between evaluations, data, and models (including preequilibrium)			
23	Collect all available experimental data - including Kammerdiener's data and Baba's (U8) data			
24	Review various theoretical approaches, as embodied in codes (including preeq, HF, Coupled Channels, KKM, PFNS background, ...)			
25	Discuss and review optical model options			
26	Seek consensus on best evaluated representation of data - including possible continued use of pseudostates			
27	Understand implications from integral data testing on changes in inelastic scattering - especially 14 MeV pulsed spheres/transmission data			
28	Assess covariances and implement in ENDF format			
29	Create ENDF formatted files			
30	Neutron Capture			
31	239Pu: Review discrepancies between evaluations, which exceed 10% at the higher energies			
32	235U: Review discrepancies between evaluations, which exceed 25% near 1 KeV (Japan's higher result) and 10% at the higher energies			
33	238U: Consider adopting 238U capture from standards - ENDF/B-VII used this, but with some small differences. Study implications from data testing of			
34	238U: Monitor Standards results for any changes, based on new measurements from DANCE, nTOF, Geel			
35	239Pu: Review data (very few measurements, especially above 100 keV there is just the LANL Hopkins data); See if DANCE data is available in time			
36	235U: Review new DANCE data and RPI data, that appear to corroborate JENDL changes near 1 keV, but point to higher energy changes too			
37	Review guidance from integral PROFIL data (suggests PU9 and (maybe) U5 from ENDF should be higher), and Wallner AMS data at 25 keV and 420 keV			
38	Assess model calculations predictions (consistent with above inelastic scattering HF/CC/OM calculations)			
39	Seek consensus on best evaluated representation of data			
40	Understand implications from integral data testing on changes in capture - especially k-eff and reaction rates (spectral indices for 85/5f etc)			
41	Assess covariances and implement in ENDF format			
42	Create ENDF formatted files			
43				
44	n2n			
45	Discuss data, including discrepancies in rise from threshold, and differences near 14 MeV			
46	Review existing evaluations (including "GEANIE evaluation" for 239Pu), data, and calculation predictions			
47	235U: New (n,xng) data to be published in PRC by Kerveno et al. (IPHC, Strasbourg (F)) could be useful to model n2n scattering, see prelim results in f			
48	239Pu: Carefully note insights on n2n making 238Pu from LANL, and discuss contradictory feedback from PROFIL			
49	Validate any changes against n,2n reaction rates in critical assemblies, eg Fig 57 in NDS112,(2012) ENDF			
50	Create ENDF file and covariances			

71	Fission (all energies), cross sections, nubar and spectra for n,g		
72			
73	Review Overall Goals, as embodied in this document and in LAUR CIELO document		
74	Fission Cross Section		
75			
76	Seek consensus that we adopt the fission cross section standard from the IAEA group		
77	Assess implications of adopting standard fission cross section on integral testing		
78	If IAEA standards team updates their value, use it; this would include any recent/forthcoming fission measurements, eg nTOF, RPI, TPC		
79	Modeling of fission would occur as part of the above inelastic/capture/n2n activities, but seek consensus that we do not use calculations in th		
80			
81	238U:Subthreshold fission for 238U – discrepancies between different evaluations. Lead spectrometer measurements near 70 keV suggest a p		
82	prompt nubar		
83	Review existing evaluations and experimental data, & review various theoretical approaches; 238U low energy interp fix needed in ENDF		
84	Seek to use an "unadjusted" nbar in a final evaluation, avoiding the ENDF "tweal" near an MeV that was adopted to better match Jezebel, Go		
85	Study Koning-Rochman nubar near thermal, from their optimization search (but it's 3 SD below the standards constants value)		
86	Develop a new evaluation based on a covariance analysis of the data		
87	Understand implications from integral data testing on changes in nubar - especially k-eff		
88	Create ENDF formatted files, including covariances		
89			
90	PFNS		
91	Review work of IAEA CRP on PFNS		
92	Aim to adopt the CRP's recommendation		
93	Seek consensus on using LANL high-accuracy NUEX Pu9 and U5 data, as published in Dec NDS2011 to help define high-energy spectrum		
94	Use new PFNS measurements, especially below MeV, coming from LANSCE/Chi-nu in the coming years		
95	Use guidance on high energy tail of spectrum from dosimetry reactions (new IAEA IRDFF CRP), eg from LANL crits, Russian fast reactor, & CE		
96	As part of IAEA CRP, advance our theoretical models, and use incorporate other data (new and existing)		
97	Understand implications from integral data testing on changes in inelastic scattering - especially k-eff and reaction rates in assemblies		
98	Create ENDF formatted files, including covariances		
99			
100	PFGS		
101	Review existing evaluations and experimental data, and various theoretical approaches		
102	Represent fission gammas separately at all energies, including above 1.09 MeV for U5 and Pu9 (an ENDF drawback), & use new data availabl		
103	Update PFGS spectra to use modern measurements from DANCE, as well as multiplicity distribution if possible		
104	Create ENDF formatted files, including covariances		
105			
106	Delayed data		
107	Review differences in present evaluatiosn		
108	Develop plan for work needed		
109			
110	Energy Release		
111	Compare energy release data in evaluations, for prompt n, g, fission fragments; and delayed energy release		
112	Update as necessary - eg ~ MeV level changes are implied for 239Pu from Jandel's DANCE data for 239Pu (but 235U looks good)		
113	Consider updating energy release incident-energy-dependence based on Lestone's work		
114			

116	<b>Integral Data Testing and Validation</b>		
117			
118	Review Overall Goals, as embodied in this document and in LAUR CIELO document		
119	Define suite of critical assembly, reactor, transmission, etc experiments to use in validation assessments, and observables (k-eff, rates, spectral indices)		
120	238U: selection of 12 ICSBEP criticality benchmarks sensitive to elastic scattering is available from JSI/IAEA (Trkov, Capote)		
121	Seek to ensure good performance in data testing, which includes:		
122	Fast, intermediate, and thermal assemblies, k-eff		
123	239Pu: Aim for (Partial?) improvement of longstanding overprediction of thermal Pu solutions		
124	Modeling spectral indices well in various systems (incl fast), 8f/5f, 9f/5f, 237np-f/5f, 233u-f/5f etc, see Table XXXVIII in VII.1 NDS 2011 paper		
125	Modeling of post irradiation experiments (PIE) such as PROFIL (CEA) and MANTRA (INL)		
126	Modeling MOX experiments for mock up of LWR, eg in EOLE, Cadarache		
127	See if PFNS improvements give improved n2n detector responses in fast crits, eg through a softer PFNS spec above 10 MeV		
128	nubar validation using multiplication subcritical measurements		
129	LLNL pulsed spheres		
130	Can we obtain improved predictions of intermediate assemblies, eg ZPR at Argonne		
131	Aim to maintain good prediction of crits, including new as-built high-resolution 3D MCNP Jezebel model?		
132	Use sensitivity methodologies for assessing changes/improvements by reaction and energy range		
133			
134			
135			
136			
137			

# Pu-SOL-THERM Benchmarks – I. Prelim LANL testing of new Subgroup 34 resonance results

- **A ~500 pcm bias in calculated PST reactivity is a long-standing issue.**
- **WPEC Sub-Group 34 was tasked with defining a new (better?) set of resolved resonance parameters for  $^{239}\text{Pu}$  in an attempt to resolve this issue.**
- **Can define a sub-set of these 150 benchmarks to test revised data files.**



- *Consider benchmark attributes such as (i) ATLF; (ii)  $^{239}\text{Pu}$  atom-% in Pu; (iii) Above-Thermal Fission Fraction (ATFF); (iv) H/Pu number density (or gPu per liter) to define this sub-set.*

## Pu-SOL-THERM Benchmarks – II. Prelim LANL testing of new Subgroup 34 resonance results

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- **A set of seven Pu-SOL-THERM benchmarks have been extracted from the larger set.**
  - PST1.4 & PST12.13 span the ATLF space;
  - PST12.10 & PST34.15 span the ATFF space;
  - PST4.1 & PST18.6 span the  $^{239}\text{Pu}$  atom percent space;
  - PST12.10 & PST34.4 span the g Pu per liter space.
- **All benchmark experiments are performed in simple geometry**
  - PST1.4 & PST4.1 are a water-reflected spheres;
  - PST18.6, PST34.4 & PST34.15 are water-reflected cylinders;
  - PST12.10 & PST12.13 are a water-reflected slabs;

# Pu-SOL-THERM Benchmarks – III. Prelim LANL testing of new Subgroup 34 resonance results

• The E71 1.00576  $k_{calc}$  average demonstrates that the 7 benchmark subset reflects the larger population.

• Data revisions in the “Leal7a”  $^{239}\text{Pu}$  evaluated file have eliminated ~50% of the long-standing  $k_{calc}$  bias.

**Calculated Eigenvalues<sup>(a)</sup> for a Selection of PST Assemblies  
Using Various  $^{239}\text{Pu}$  Cross Sections**

Assembly	ENDF/B-VII.1	JEFF-3.1.2 <sup>(b)</sup>	JENDL-4.0 <sup>(b)</sup>	Leal7a <sup>(c)</sup> + e71	Leal7a (RR, nu, pfns only) + e71
PST1.4	1.00448	1.00127	1.00588	1.00199	1.00202
PST4.1	1.00383	0.99907	1.00482	1.00044	1.00044
PST9	1.01939	1.01367	1.02510	1.01543	1.01546
PST12.10	1.00412	0.99973	1.00498	1.00083	1.00080
PST12.13	1.00955	1.00468	1.01069	1.00611	1.00620
PST18.6	1.00472	1.00153	1.00557	1.00202	1.00208
PST34.4	1.00258	0.99999	1.00417	0.99922	0.99937
PST34.15	0.99742	0.99563	0.99844	0.99679	0.99707
<b>Average</b>	<b>1.00576</b>	<b>1.00195</b>	<b>1.00746</b>	<b>1.00285</b>	<b>1.00293</b>
<p>a) MCNP calculations are for 250M histories; stochastic uncertainty is ~5 pcm.                      b) JEFF-3.1.2 and JENDL-4.0 <math>^{239}\text{Pu}</math> only; remaining nuclides are ENDF/B-VII.1                      c) “LEAL7a” evaluation provides revised resolved resonance parameters coupled to a joint ORNL/CEA evaluated <math>^{239}\text{Pu}</math> file; the “LEAL7a (RR,nu,pfns)” file couples just these data to the existing ENDF/B-VII.1 <math>^{239}\text{Pu}</math> file.</p>					

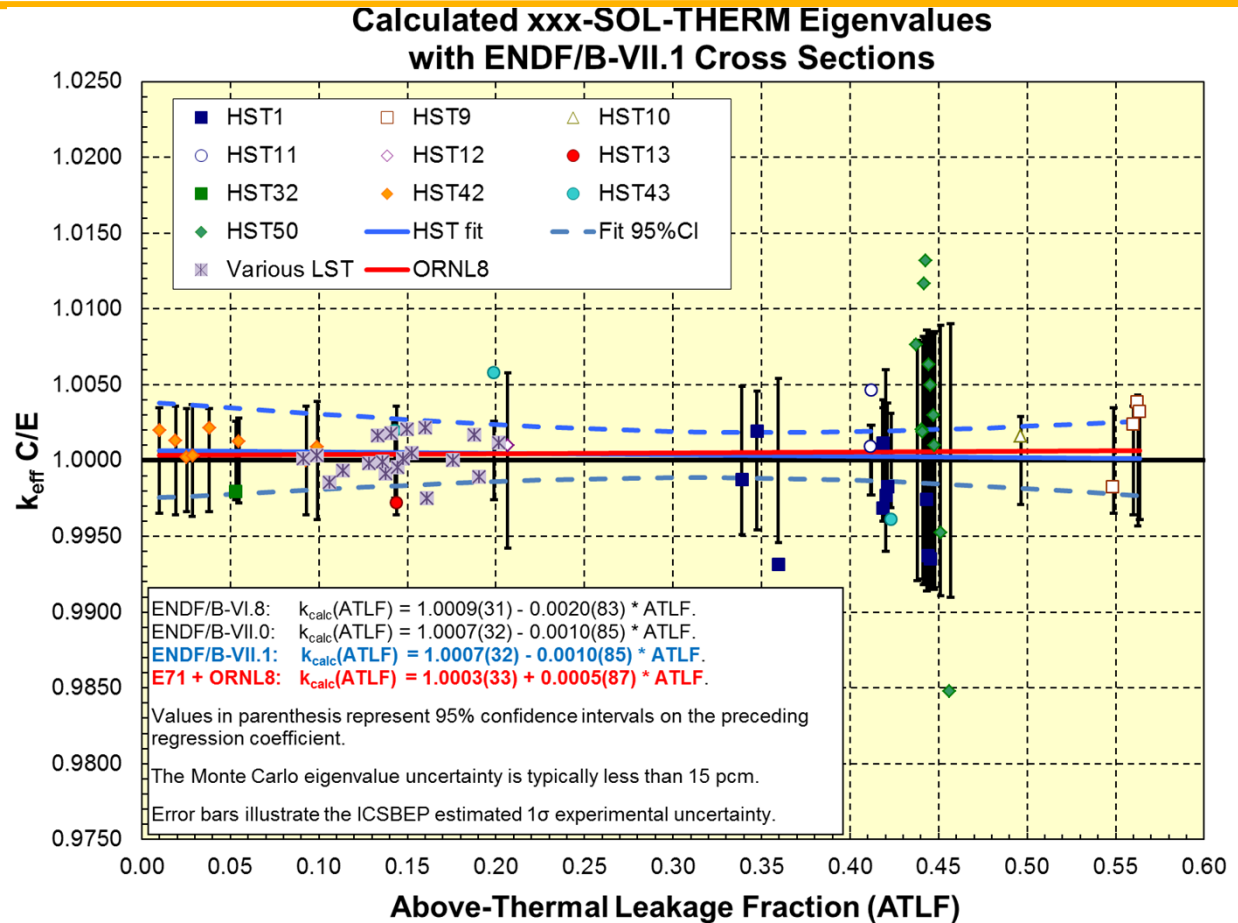
## Time-line

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- **May 2013: CIELO WPEC Subgroup initiated**
  - Teams identified
- **Nov 2013: NEMEA7-CIELO: Main collaboration kick-off**
  - Refine scope of work, collaborators who will work on tasks
  - Will result in detailed work plans, time line goals, for each nucleus
- **Next 2.5 Years:**
  - Various collaboration meetings, continual email collaborative exchanges
  - engagement with validation data testers continually
  - Incorporate new IAEA standards results (fission, capture, scattering, ...)
  - Explore interdependencies on criticality from the 6 CIELO nuclides
- **May 2016:**
  - Document conclusions from CIELO collaborations in WPEC report (& NDS paper?)
  - Create formatted files that embody CIELO's initial conclusions

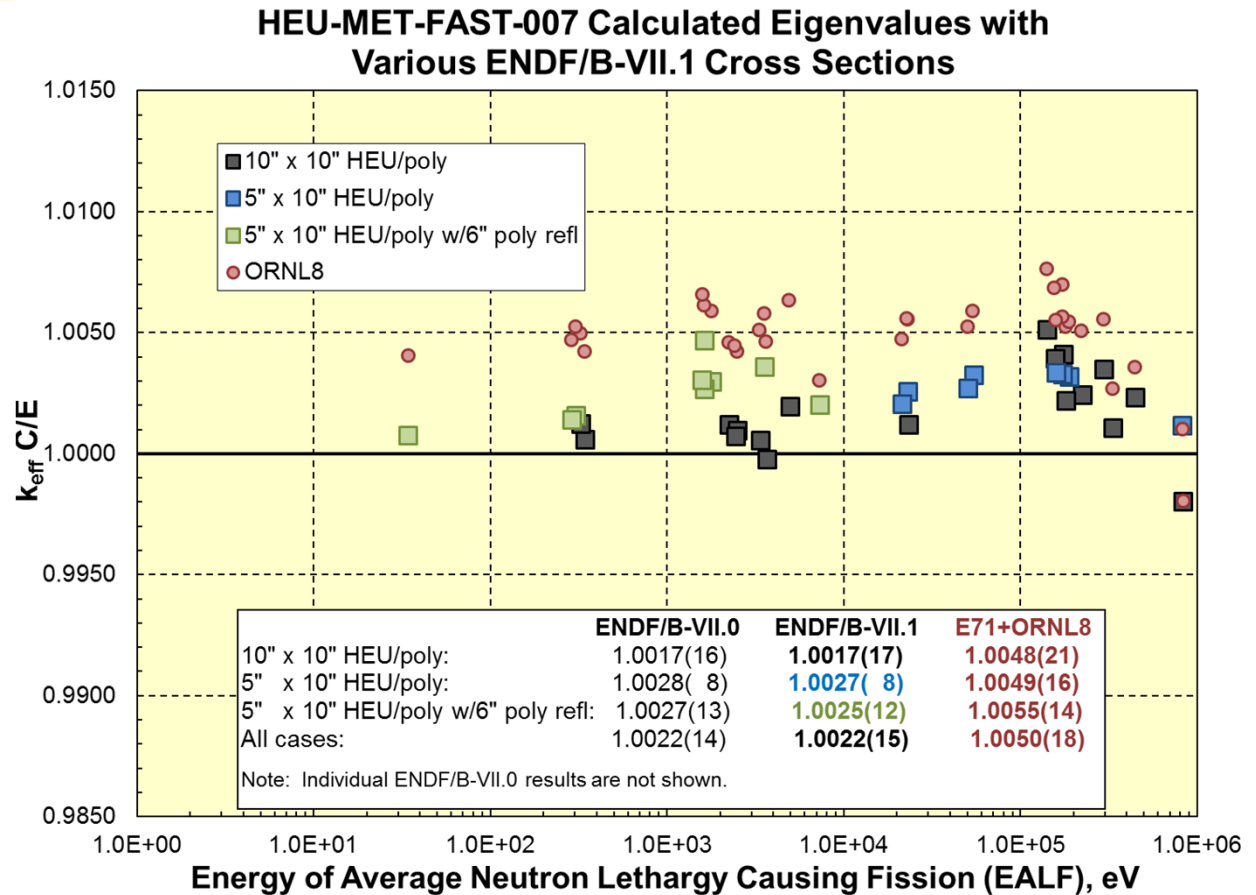
# HST Benchmarks - LANL testing of prelim Res file

- Regression fit to HST benchmarks versus ATLF has been excellent since ENDF/B-VI.3 (Lubitz).
- This excellent fit is retained with the latest **(ORNL8)** <sup>235</sup>U resolved resonance file.



# HMF7 (HEU + CH<sub>2</sub>) : LANL testing of prelim Res file

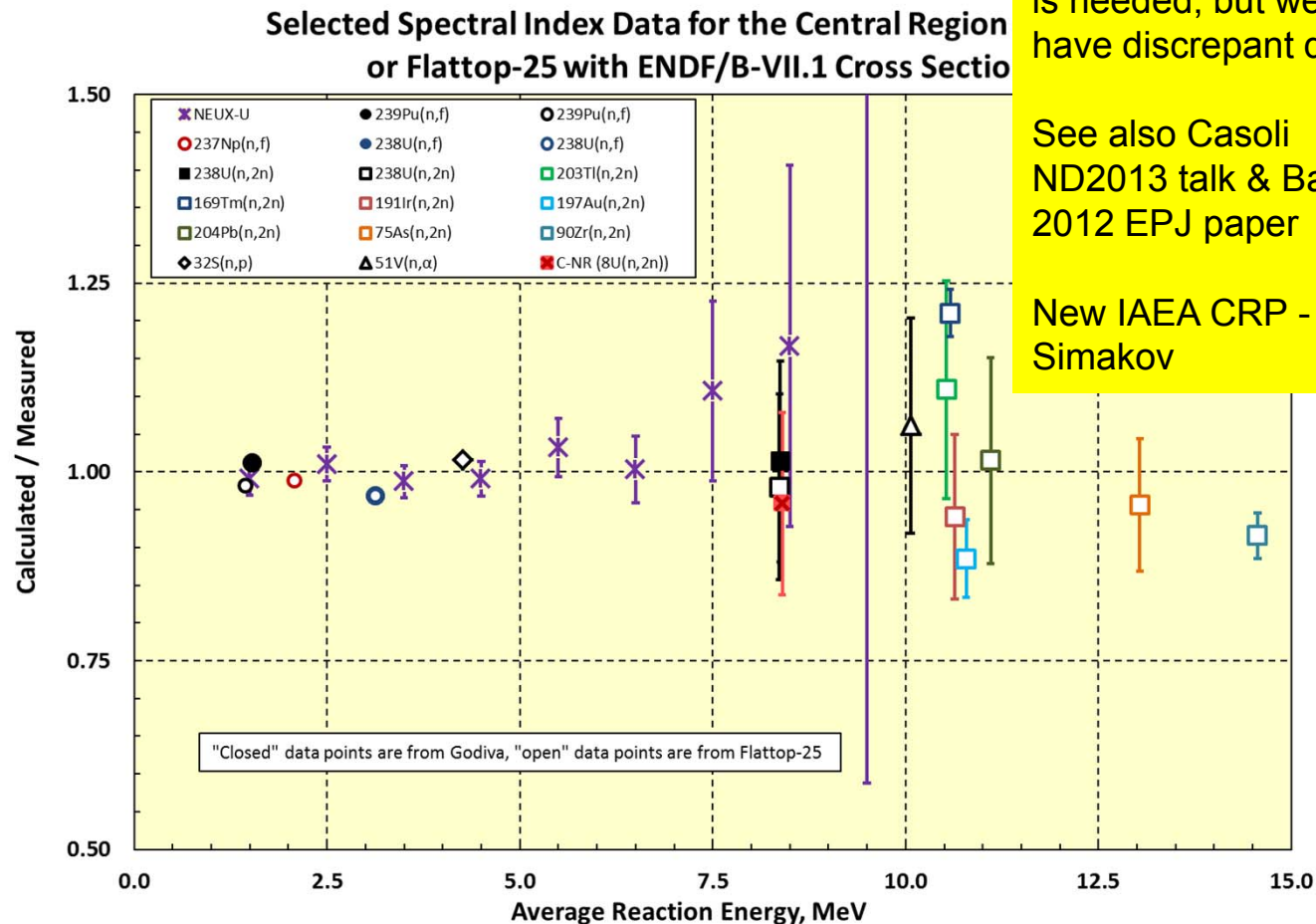
- HEU + poly system tests xs data over several orders of magnitude.
- E70 & E71 results are near unity at either energy extreme but are biased high in the intermediate energy range.
- This bias is worsened with the latest ORNL8 <sup>235</sup>U evaluated file.



# Reaction Rates in Fast Critical Assemblies Provide Integral Test of Prompt Fission Neutron Spectrum & (n,2n) Cross Sections - Uranium-235 data

<sup>235</sup>U

With NUEX data added (Lestone)



Perhaps suggests a softer ENDF spectrum is needed, but we have discrepant data.

See also Casoli ND2013 talk & Bauge 2012 EPJ paper

New IAEA CRP - Simakov

Similar analysis for plutonium systems – see our ND2013 proceedings paper

# More Data Testing on Preliminary 235U ORNL Res File

$k_{calc}$  Summary for Various Benchmarks and Cross Section Data Sets

GODIVA (HEU-MET-FAST-001)		
Cross Section Set	Benchmark $k_{eff}$	$k_{calc}$
ENDF/B-VII.1	1.000(1)	0.99983(3)
E71 + ORNL8		0.99985(2)
J4 + ORNL8		0.99757(2)
CEA + ORNL8		0.99957(2)
Flattop-25 (HEU-MET-FAST-028)		
ENDF/B-VII.1	1.0000(16)	1.00285(2)
JENDL-4.0		0.99779(9)
E71 + ORNL8		1.00300(13)
J4 + ORNL8		0.99899(13)
CEA + ORNL8		1.00040(13)
Big-10 (IMF7, detailed model)		
ENDF/B-VII.1	1.0045(7)	1.00443(2)
JENDL-4.0		0.99710(7)
E71 + ORNL8		1.00471(8)
J4 + ORNL8		0.99764(11)
CEA + ORNL8		0.99901(11)

## More Data Testing on Preliminary 235U ORNL Res Rile

3

	HMI6.1	HMF6.2	HMI6.3	HMF72.3	HMI6.4	HMF72.1	HMF73
Benchmark $k_{eff}$	0.9977(8)	1.0001(8)	1.0015(9)	1.0016(69)	1.0016(8)	0.9991(24)	1.0004(16)
<u>endf/b-vii.1 ealf</u>	4.93 keV	10.1 keV	23.5 keV	40.8 keV	79.8 keV	223 keV	416 keV
	$k_{calc}$						
ENDF/B-VII.1	0.99293(2)	0.99690(2)	1.00076(2)	1.01236(2)	1.00730(2)	1.00852(1)	1.00807(2)
ENDF/B-VII.1 + e5 <sup>nat</sup> Cu	0.99264(2)	0.99723(2)	1.00168(2)	1.00762(10)	1.00767(2)		0.99663(2)
ENDF/B-VII.1 + <u>mit/ornl</u> <sup>63,65</sup> Cu	0.99304(15)	0.99709(15)	1.00086(15)	1.01254(10)	1.00791(15)		1.00720(14)
JENDL-4.0	0.99810(11)	1.00197(11)	1.00428(11)		1.00569(10)		1.00267(9)
E71 + ORNL8	1.00188(2)	1.00616(2)	1.00929(2)	1.01744(10)	1.01196(2)	1.00921(9)	1.00809(1)
J4 + ORNL8	0.99629(2)	0.99987(2)	1.00226(2)		1.00451(2)		1.00276(2)
CEA + ORNL8	0.99578(2)	0.99922(2)	1.00149(2)		1.00390(2)		1.00361(1)

JENDL-4.0 is <sup>iso</sup>U only; remaining cross sections are endf/b-vii.1.

J4+ORNL8 is the <sup>235</sup>U data set; remaining cross sections are endf/b-vii.1.

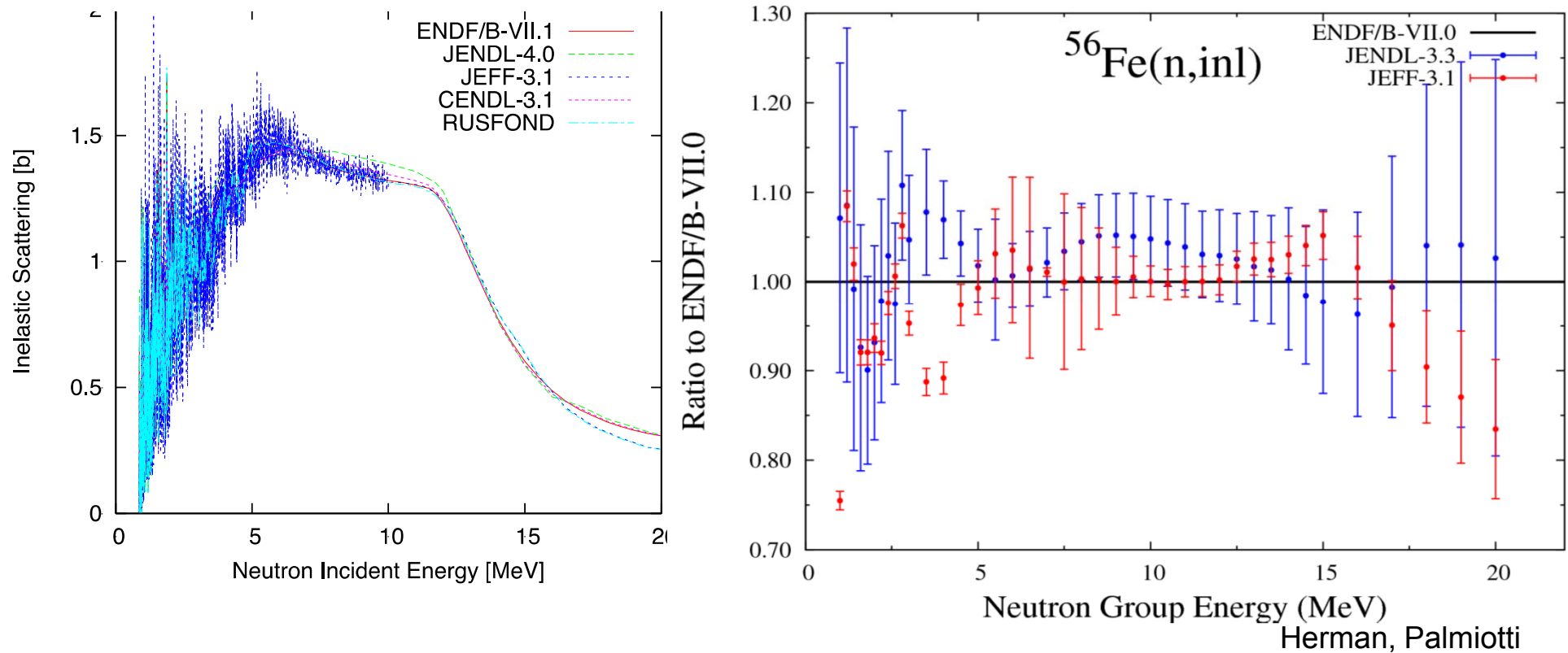
$k_{calc}$  values with a ~2 pcm uncertainty were run for 2 billion histories and include detailed multigroup tallies.

HMI6 has varying amounts of interstitial carbon; HMF72.1 has interstitial carbon steel (Fe); HMF72.3 has interstitial carbon steel (Fe) and polyethylene; HMF73 is HEU only ... all assemblies are surrounded by a thick copper reflector (i.e., HMI6, HMF72 and HMF73 are different flavors of ZEUS).

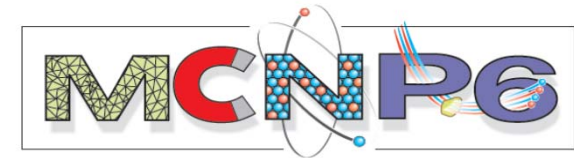
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2		
3	<b>56Fe</b>	
4		
5		
6		
7	General	
8		Review differences in evaluations. In ENDF/B-VII.1 RR extend up to 850 keV, but pointwise fluctuations extend up to almost 10 MeV.
9		Get insights from previous evaluators on tasks to work on. For example, Trkov, Koning, Vonach, Tagesen were involved in the last European Jeff ev
10		Optical model and other key modeling parameters
11		
12	Fast Region	
13		
14	Inelastic and elastic	
15		Review new data,: RPI has high-res transmission up to 2 MeV, and scattering data ("quasi differential data"), that needs an MCNP calc to compare
16		
17		Review new data:Arjan Plompen (Geel) has inelastic data (actually, gamma-production) too measured this year, from 800 keV to 5 MeV.
18		Review new data: Schillebeeckx and Trkov's postdoc have made some new measurements, and reviewed existing measurements....
19		Review new data: Ron Nelson (LANL) has gamma-production data for iron.
20		Review new data: The Grimes et al. Ohio work should be looked at too – it is suggesting a big change for nonelastic, but that our total cross sectic
21		IAEA coupled-channel OM work going on for iron.
22		Pronyaev – also doing work on inelastic gamma production. At one point this was being considered as a standard (now more likely to use TI).
23		
24	Charged-particle production	
25		Review data, evaluations, and model predictions for (n,alpha) etc
26		Data above 20 MeV may be needed too, eg for fusion applications, using new gas-production data from Haight.
27		
28	Activation xs	
29		Review/Include activation data needed for fission/fusion
30		
31	DPA	Take advantage of insights from new IAEA CRP on damage and DPA
32		
33	Resonance Region, Resolved and UnResolved Parameters (hundred of keVs and below)	
34		
35	RRR & UR	Review latest evaluation from Luiz Leal
36		
37	Integral validation	
38		Define suite of integral tests - critical assemblies, transmission/shielding, reactor experiments, etc
39		17 benchmarks with iron as shielding material (+8 more with stainless steel) are available in the SINBAD database
40		Compile feedback from recent testing - eg SG33, fast reactor COMARA experience, etc, Steven VDM's NDS 2012 benchmarking paper (which note:
41		Andrej Trkov has shielding benchmarks that are relevant too. The euracos benchmark for sinbad.
42		Pay attention of Fe-reflected fast critical benchmarks (+ thermal bench from CEA, e.g. PERLE experiments in EOLE)
43		Use ZPR3-54, ZPR9-34, ZPR6-10 and possibly CIRANO with reaction rate distributions
44		Use sensitivity metodologies for assessing changes/improvements by reaction and energy range
45		
46		

# $^{56}\text{Fe}$ : Advances Needed in Inelastic Scattering



New measurements (IRMM) & SAMMY analyses in resonance region; new Hauser-Feshbach analyses at higher energies



## MCNP6 Production release, 2013

- MCNP6 = MCNP5 + MCNPX + several new features
- 2 DVD set will contain 5,X & 6 + ENDF 7.1 and > 1 Gbyte of documents
- MCNP 5/X/6 Beta 2 had 2,452 copies sent out in FY12 and more than 11,000 in the last 11 years!
- See “Initial MCNP6 Release Overview” Nuclear Technology, Dec 2012

