

LA-UR-16-23112

# Status of Cross Section Progress for $^{235,8}\text{U}$ , $^{239}\text{Pu}$ , $^{56}\text{Fe}$ , $^{16}\text{O}$

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LANL

*(with CIELO collaboration)*

WPEC Subgroup 40, OECD, Paris, May 9-13, 2016

## Abstract

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Progress is described for nuclear cross section evaluations, calculations, and experimental measurements at Los Alamos and other laboratories, on  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{16}\text{O}$  and  $^1\text{H}$ , for the CIELO project at the Nuclear Energy Agency/WPEC. This includes first data from the LANSCE Chi-nu project, providing insights into the energy spectrum of fission neutrons. The net effect of various nuclear data updates is a suite of CIELO files that models criticality well, but feature an improved agreement with differential data (prompt-fission neutron spectra, time of flight experiments in the resonance region, resonance fission neutron multiplicity, quasi-differential neutron scattering data)

# Overview comments on CIELO progress

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**Progress on our understanding of  $1\text{H}$ ,  $16\text{O}$ ,  $56\text{Fe}$ ,  $235\text{U}$ ,  $238\text{U}$ , and  $239\text{Pu}$  neutron reactions:**

- a variety of different teams and approaches
- experiments & theory advanced

**A set of starter files has been created via a USA-Europe-IAEA collaboration**

- this suite of (ENDF/B-VIII.beta1) files, taken together (with a new H2O scattering kernel), appears to model integral criticality fairly well. Validation testing ongoing (including SG39 support); future refinements planned
- other CIELO collaborations will provide alternative options
- These analyses will be documented in the coming year, including journal articles in Elsevier's Nuclear data Sheets (January 2018)

# CIELO progress: Criticality Testing & files

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Much work by many on team

- various interplaying channels studied systematically by BRC

Next phase is to create:

CIELO/A files: explore the range of physics options

CIELO/B files: recommended files from project, 1 (or2) per isotope, with integral testing & down-selection of essential suite of experiments

Covariances (uncertainties)

Document all issues, areas of consensus & disagreement, in NDS 2018 big paper, also used as SG40 final report in 1 years time

# CIELO progress: Scattering (Elastic & Inelastic) for Actinides and Iron

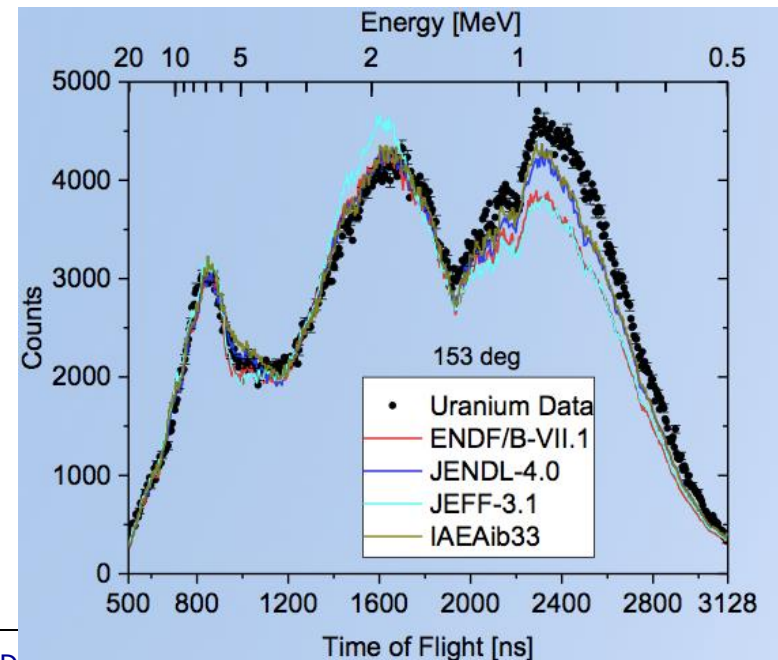
New RPI semi-integral approach has had a large impact on validating and improving inelastic and elastic scattering on  $^{238}\text{U}$  and  $^{56}\text{Fe}$

- longer term work on  $^{239}\text{Pu}$  and  $^{235}\text{U}$  planned at LANSCE

Modern inelastic scattering advances made from theory with insights from measured data:

- $^{238,5}\text{U}$  work from the IAEA
- $^{235}\text{U}$  from BRC
- $^{239}\text{Pu}$  work from LANL
- $^{56}\text{Fe}$  work from BNL, IAEA

**Note SG39 strong sens. to  $^{238}\text{U}$  inelastic**



# CIELO progress: Actinide Capture

**$^{239}\text{Pu}$ :** New LANSCE data “first” for many decades (Mosby, Jandel)

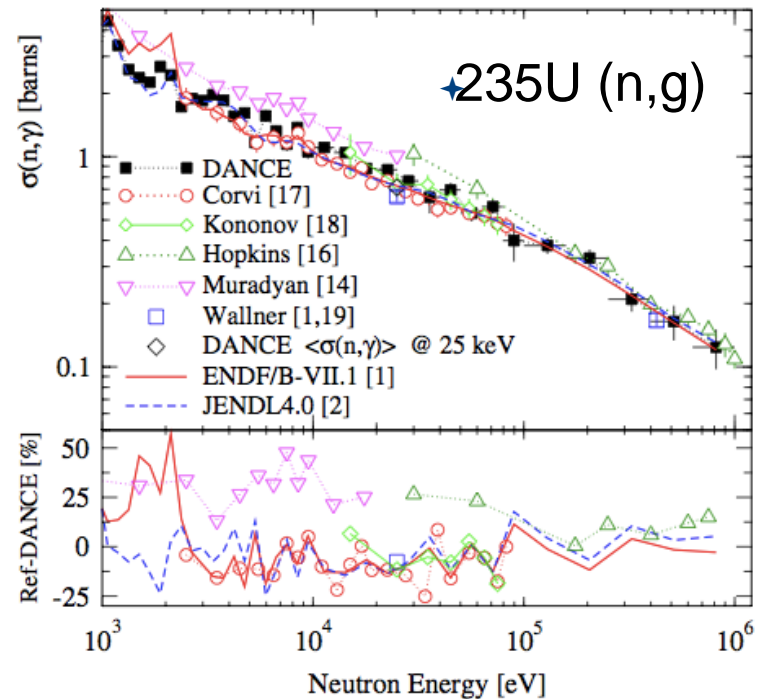
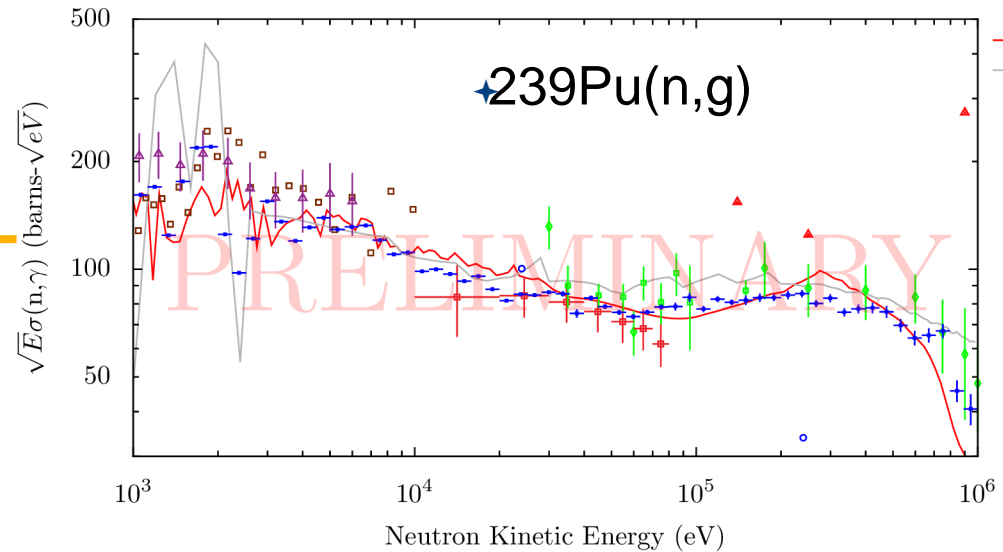
- tend to support ENDF; only modest changes needed, including above 1 keV where we need a SAMMY analyses, as for  $^{235}\text{U}$  n,g

**$^{235}\text{U}$**  was a major advance, from 0.5-2 keV (lower capture)

- In tens of keV suggests a small increase to ENDF (but contradicted by Wallner AMS measurement at 25 keV)

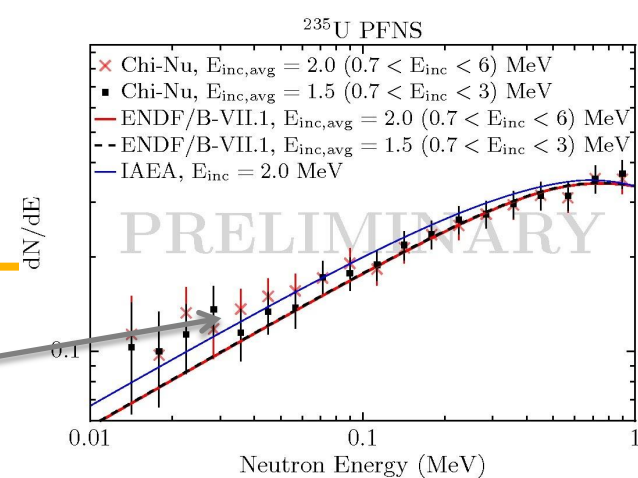
**$^{238}\text{U}$**  capture from Schbx

tends to support standards view



# CIELO progress: Actinide PFNS - Impacts everything

LANSCCE data



IAEA Standards 235U PFNS advances suggest a softer spectrum (2.00 MeV versus 2.03 average energy), but not as soft as Kornilov's 1.97

- concurrent changes to 235U nubar (lowered) being discussed

New LANSCCE PFNS from 235U supports “ENDF” Madland-Nix PFNS in the fast range near 2 MeV, as do LANL/NUEX measurements

- This challenges other studies, where softer PFNS are explored
- Leading to a view to not change fast PFNS (much, at least) for 235U and 239Pu, where Chatillon BRC/LANSCCE data also ~ supports ENDF. Chi-nu will measure 239Pu in ~ 1 years. New CIELO file uses Talou-Rising eval. For 235U

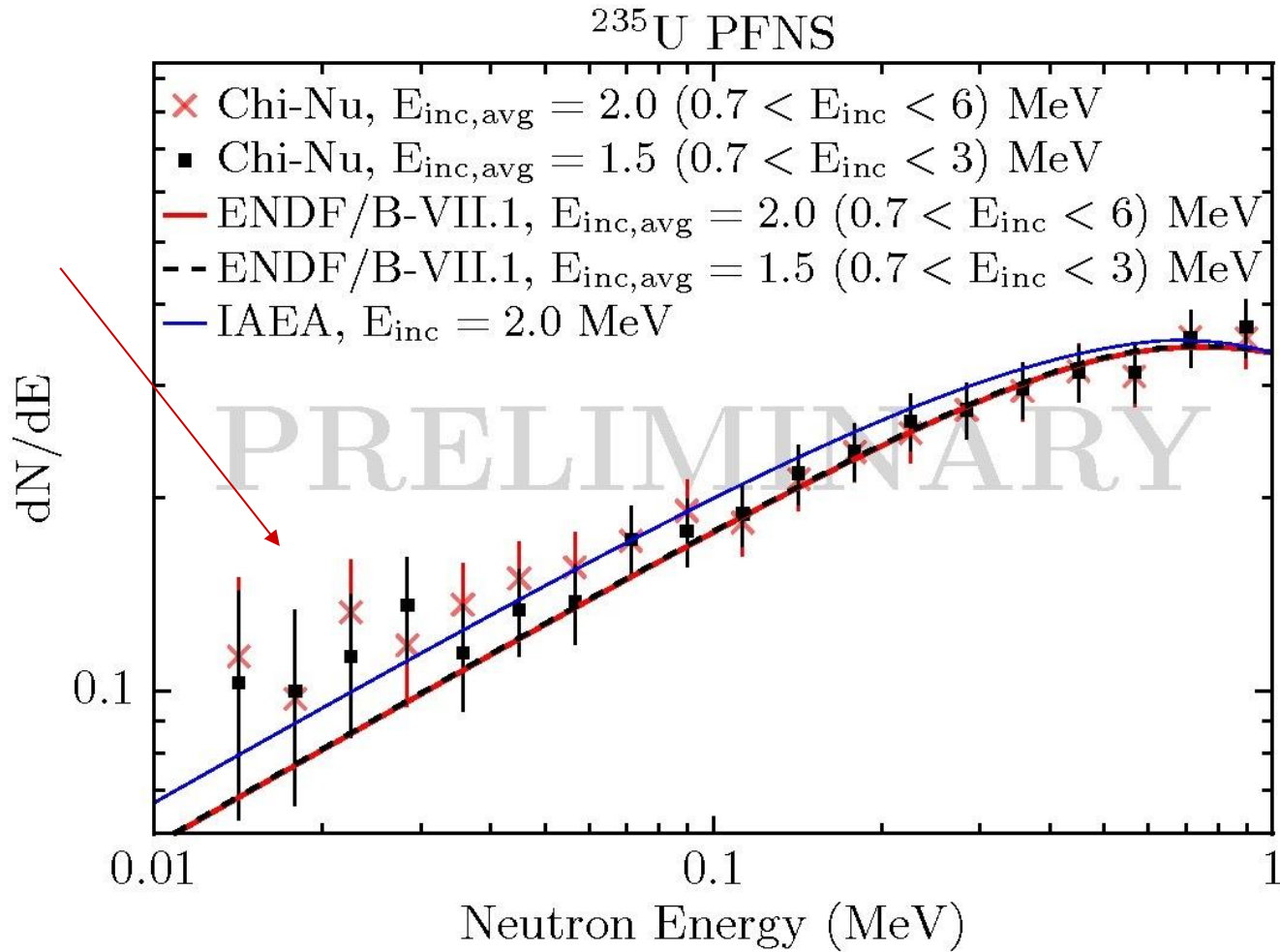
## **$^{235}\text{U}$ : LANL PFNS Experimental Work in Fast Range (0.5-6 MeV) Suggests ENDF PFNS is Accurate**

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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

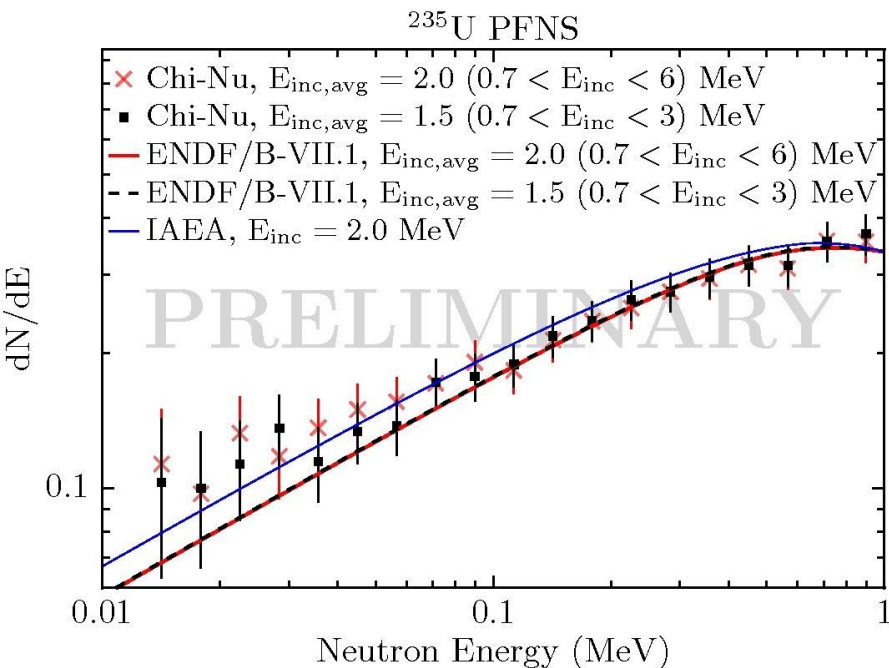
## $^{235}\text{U}$ : LANL PFNS Experimental Work in Fast Range (0.5-6 MeV) Suggests ENDF PFNS is Accurate

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)

$E_{\text{out}} < 1 \text{ MeV}$



$E_{\text{out}} > 1 \text{ MeV}$

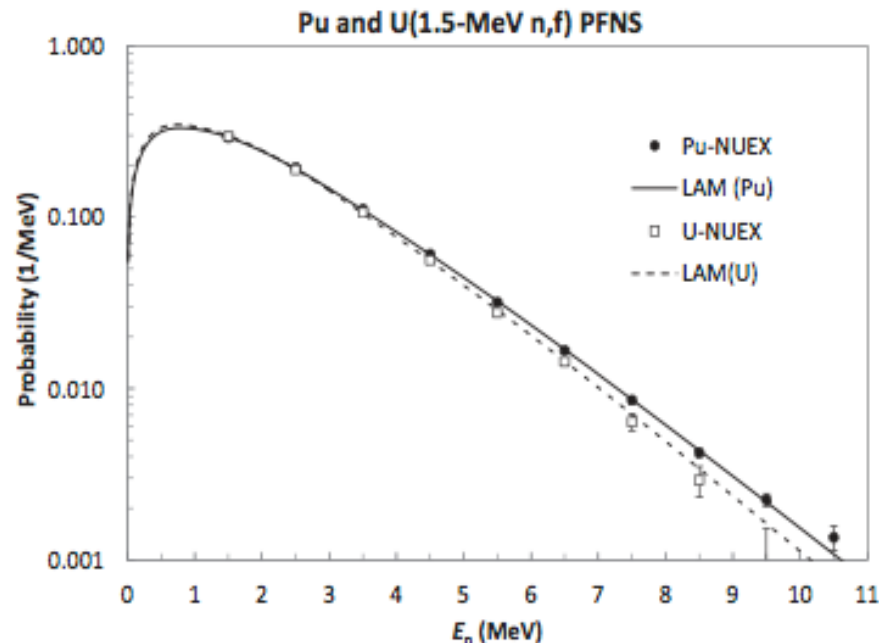


FIG. 3. The emission probabilities listed in Tables III and IV, and the corresponding 1.5-MeV  $n + ^{239}\text{Pu}$  and  $^{235}\text{U}$  Los Alamos fission model fission-neutron energy spectra (curves).

## $^{239}\text{Pu}$ : 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

# Improvements in the new LANL evaluation –

## Neudecker work

### ∅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)

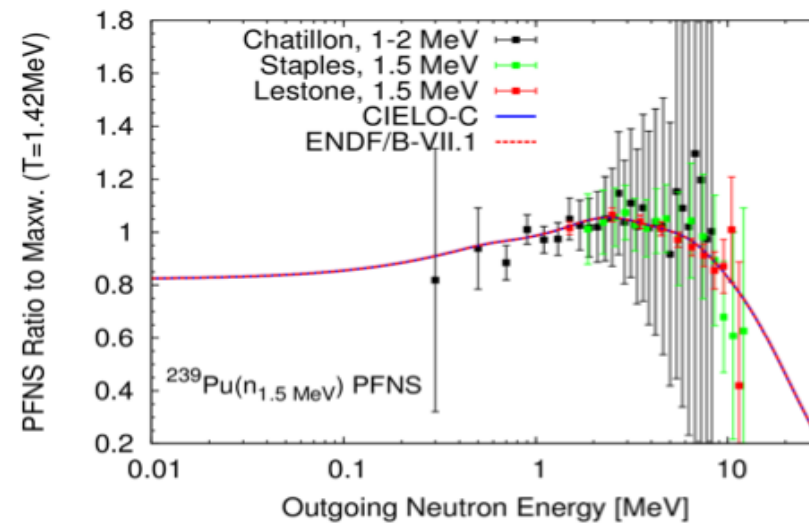
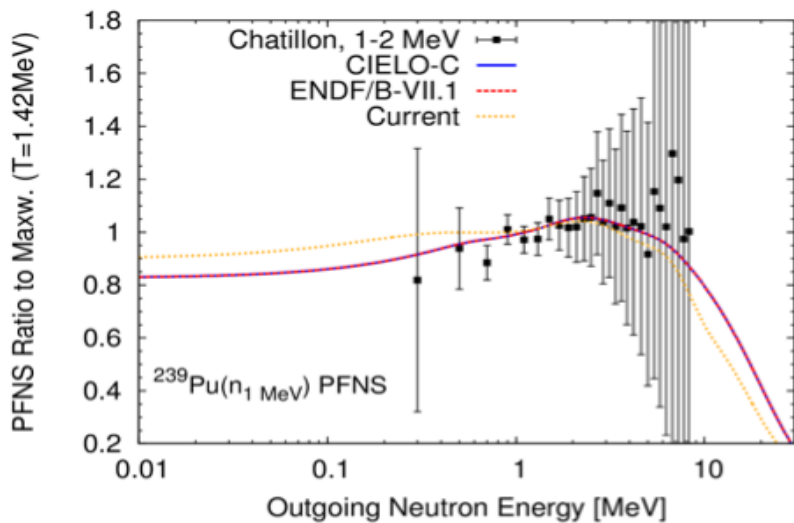
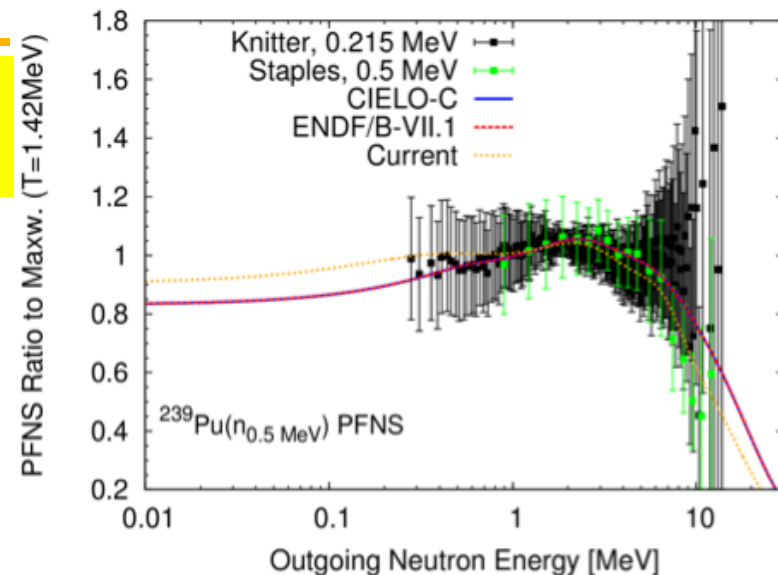
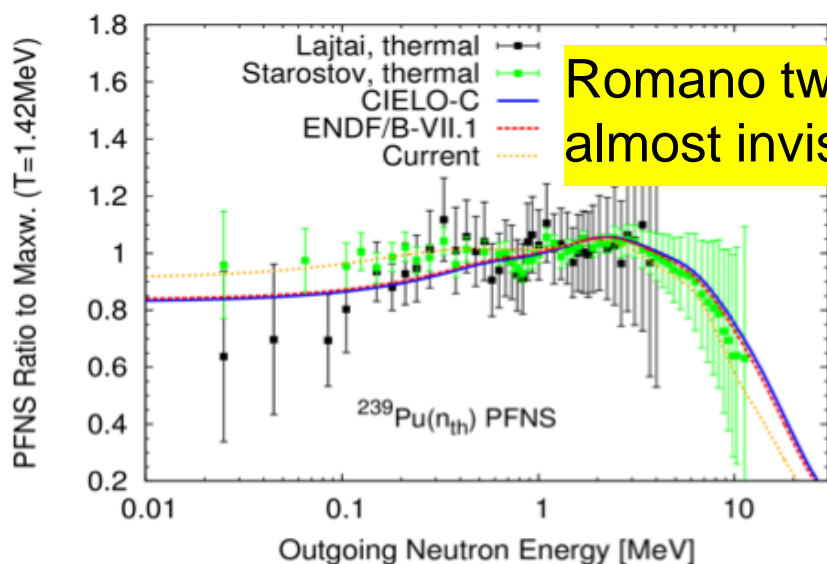
### ∅Modeling:

- ┆ Einc-dependent parametrization of  $\langle \text{TKE} \rangle$  and  $\langle \text{Er} \rangle$  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

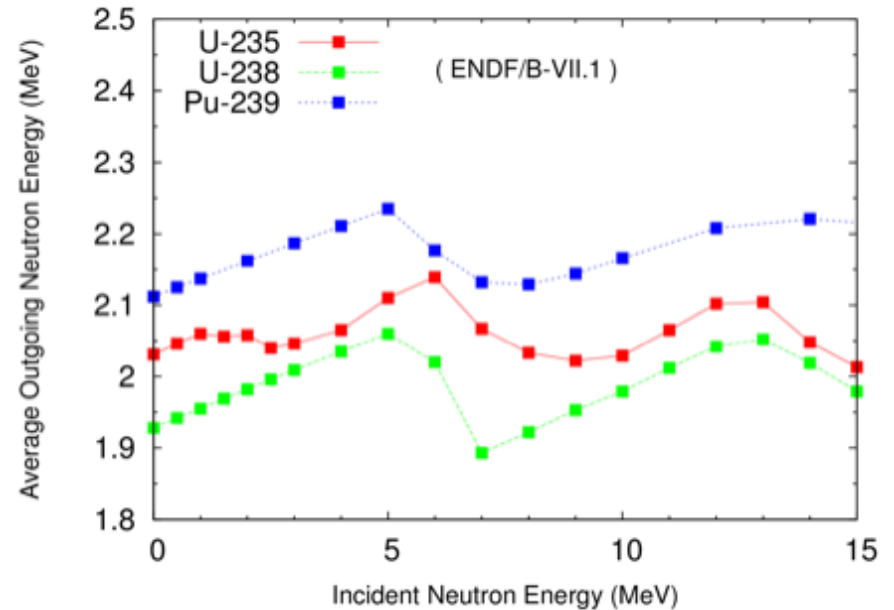
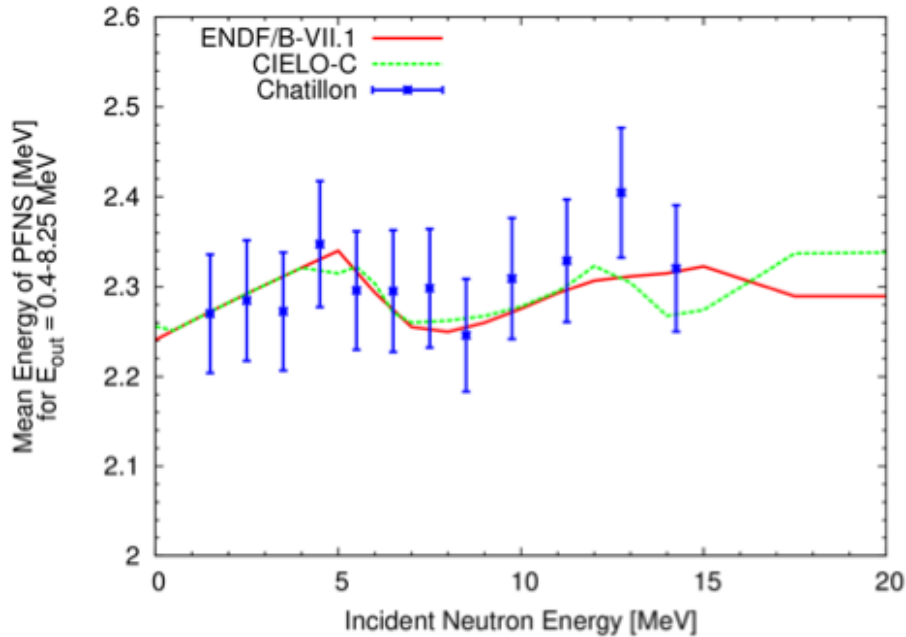
### ∅Evaluated output:

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

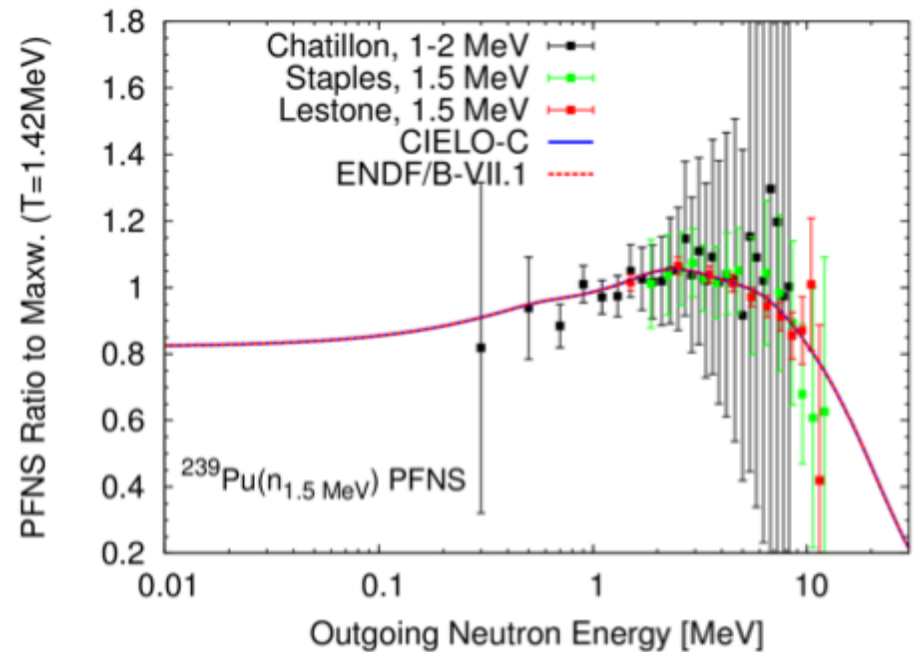
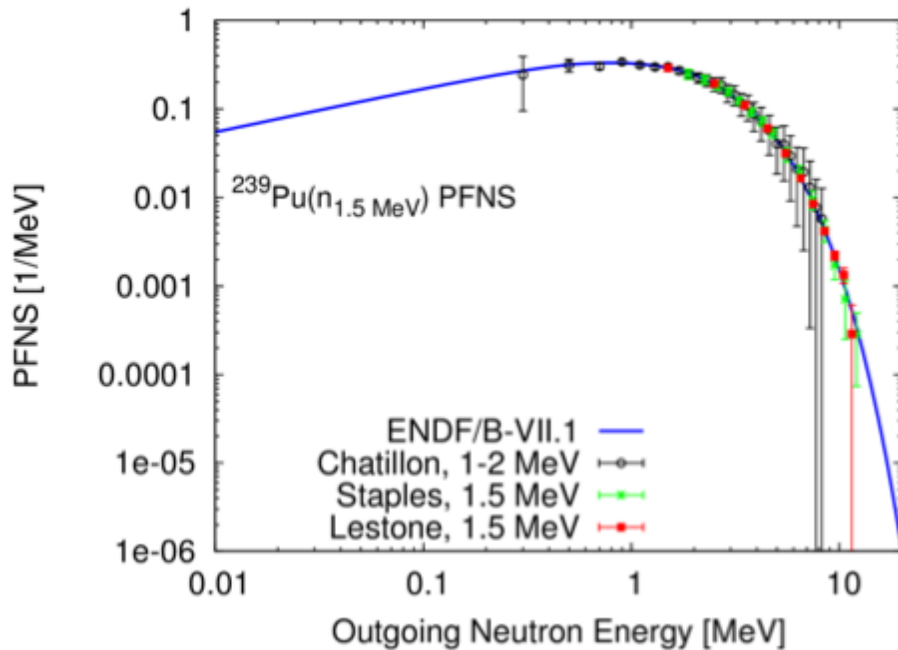
# 239Pu PFNS at all given Einc, Compared to Neudecker's Current Evaluation



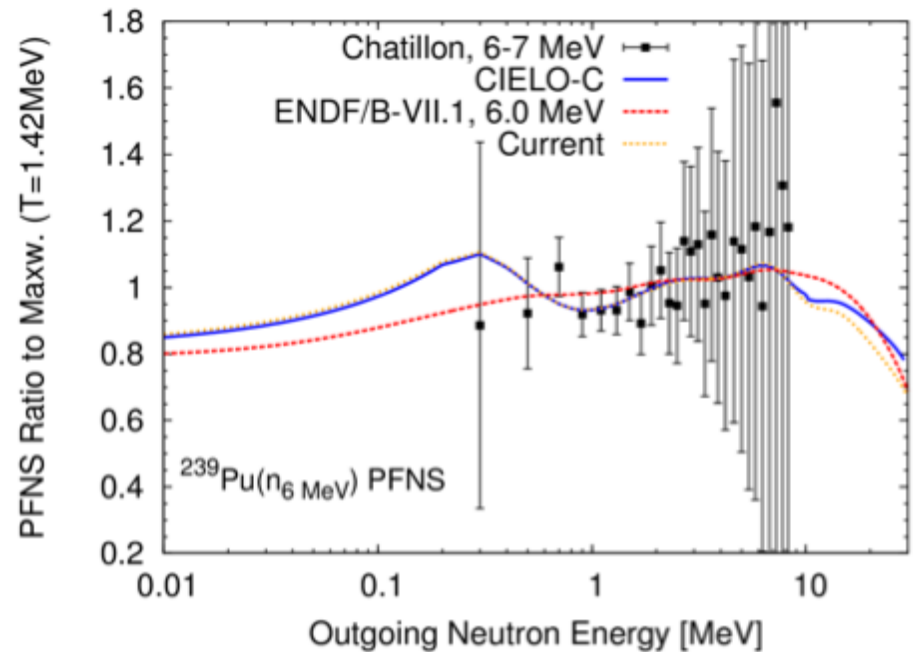
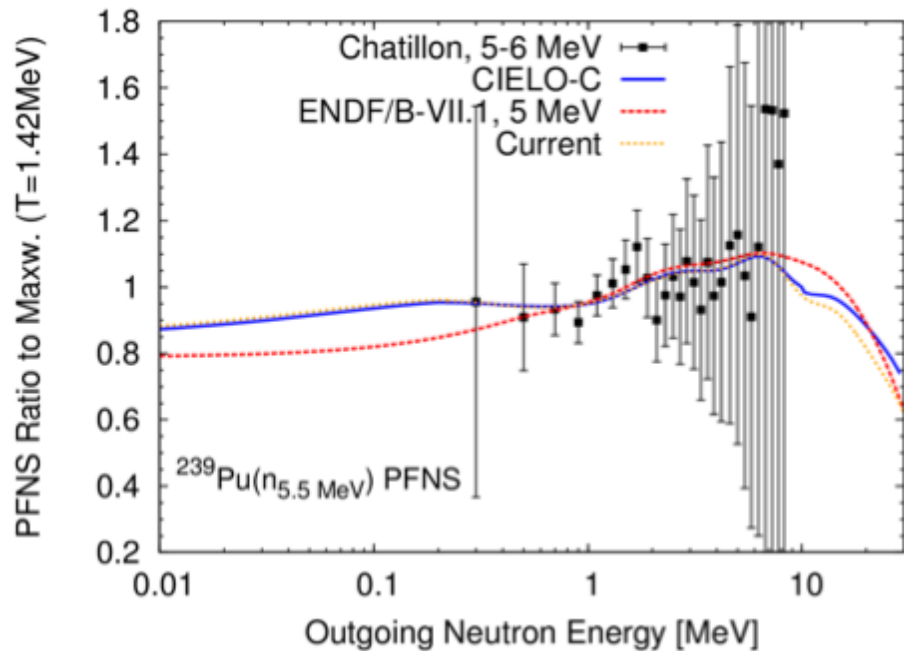
# PFNS Average Energy – CIELO file for testing (ENDF <5 MeV except for a tweak at thermal by Romano, and Neudecker > 5 MeV)



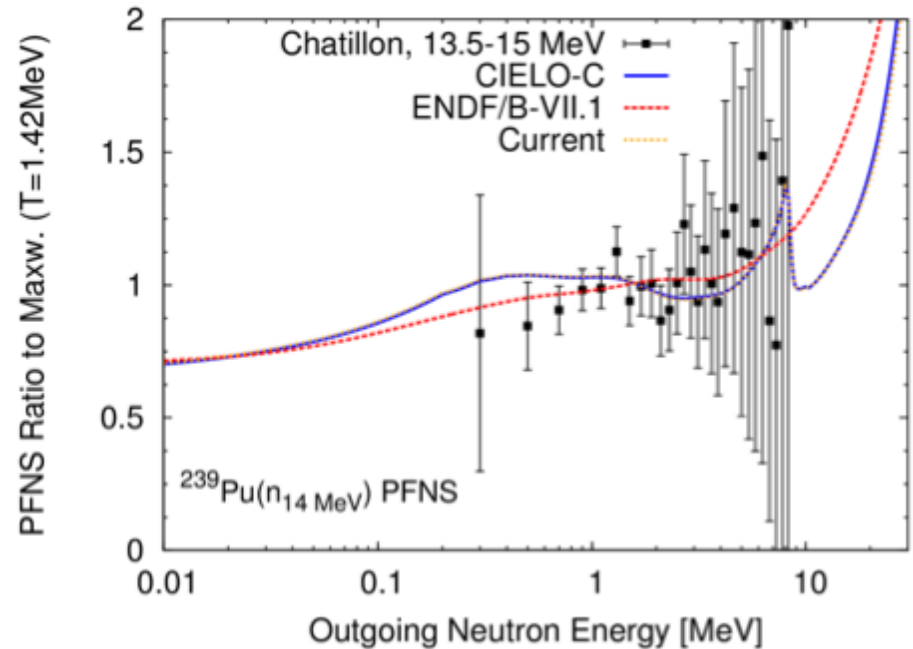
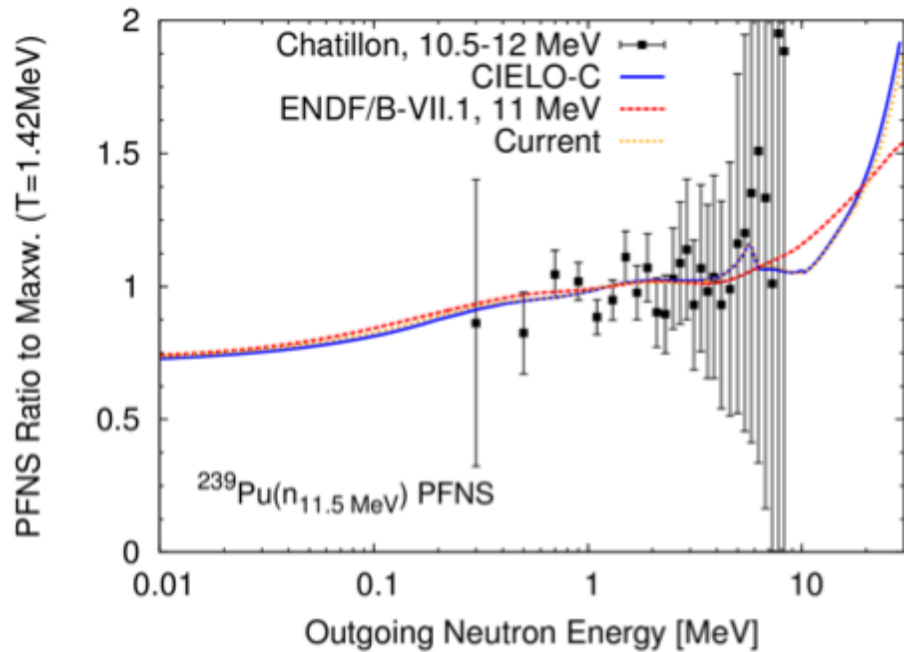
# ★<sup>239</sup>Pu PFNS at E<sub>inc</sub> = 1.5 MeV



# ★<sup>239</sup>Pu PFNS at E<sub>inc</sub> = 5.5-6 MeV (opening of second chance fission)



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

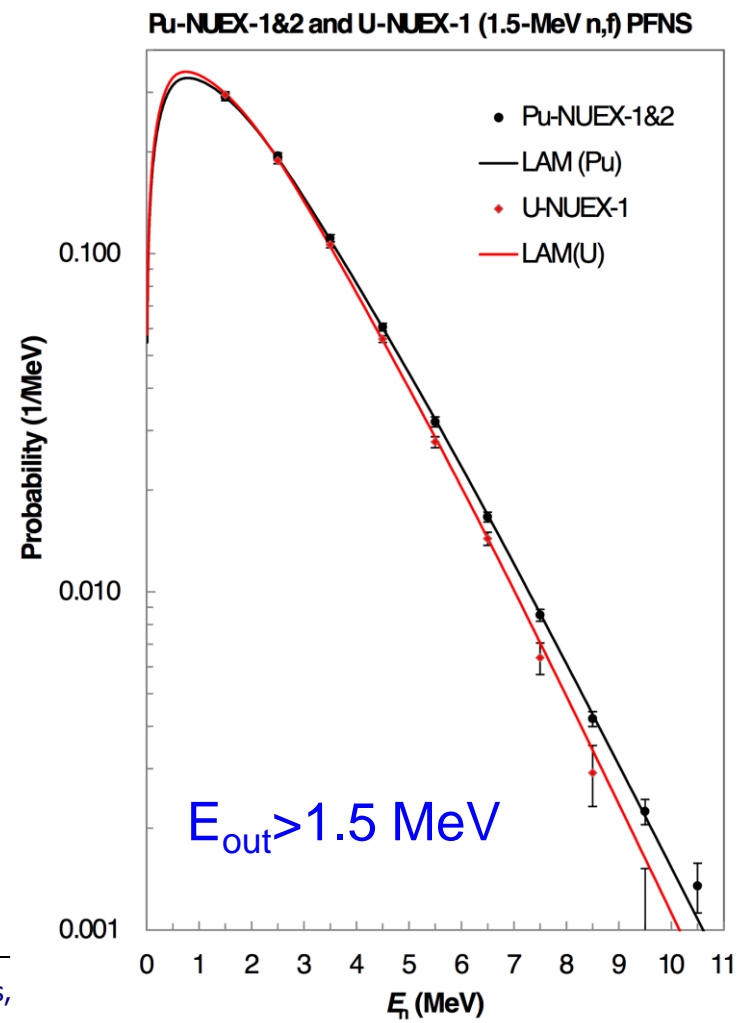
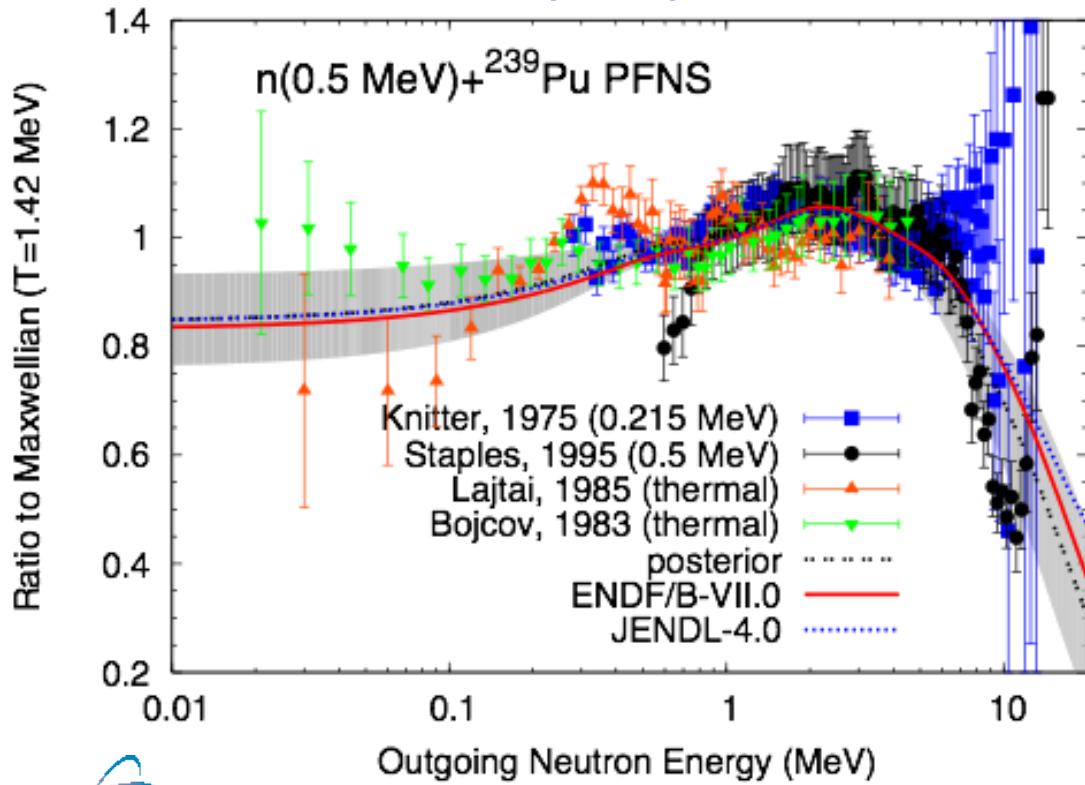


# Determining the Prompt Fission Neutron Spectrum (Chi): One of Our Highest Priorities & an IAEA CRP.

## Chi-nu PFNS delayed till next year (235U measured recently)

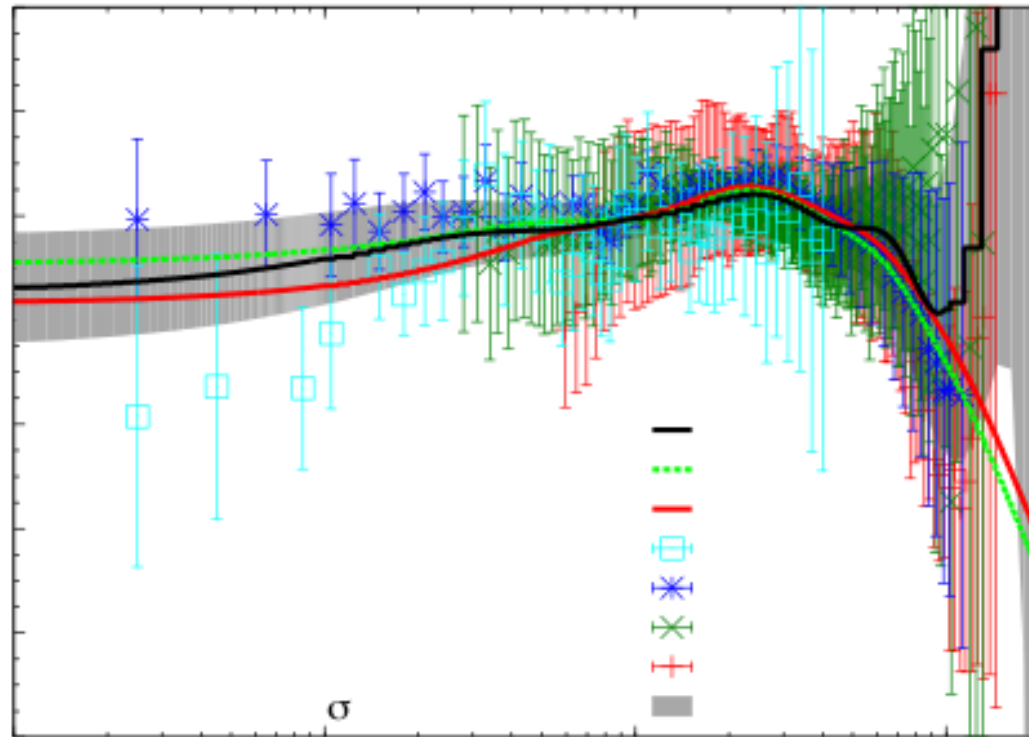
Large uncertainties below 1 MeV and above 5 MeV impact criticality calculations and (n,2n) transmutations

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



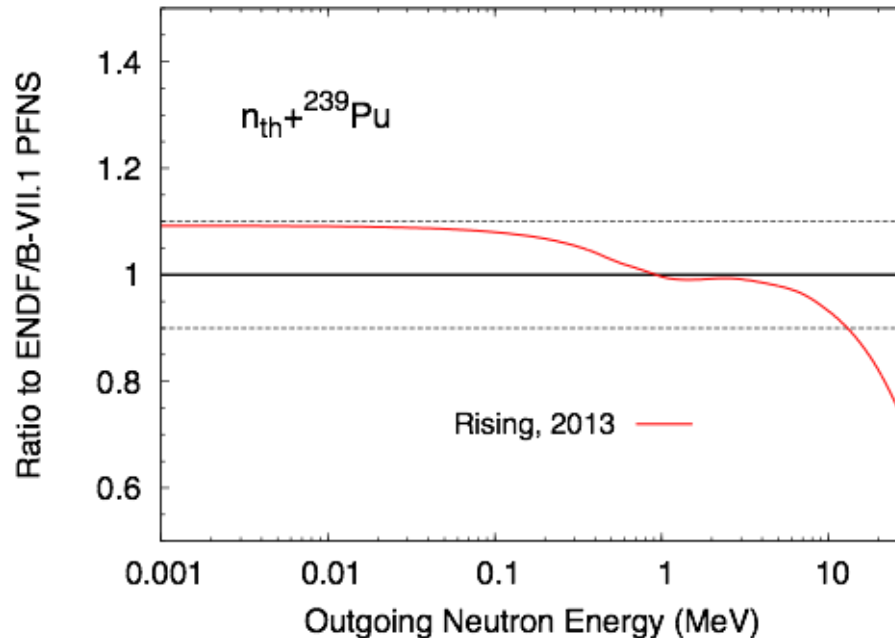
Talou, Vogt

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



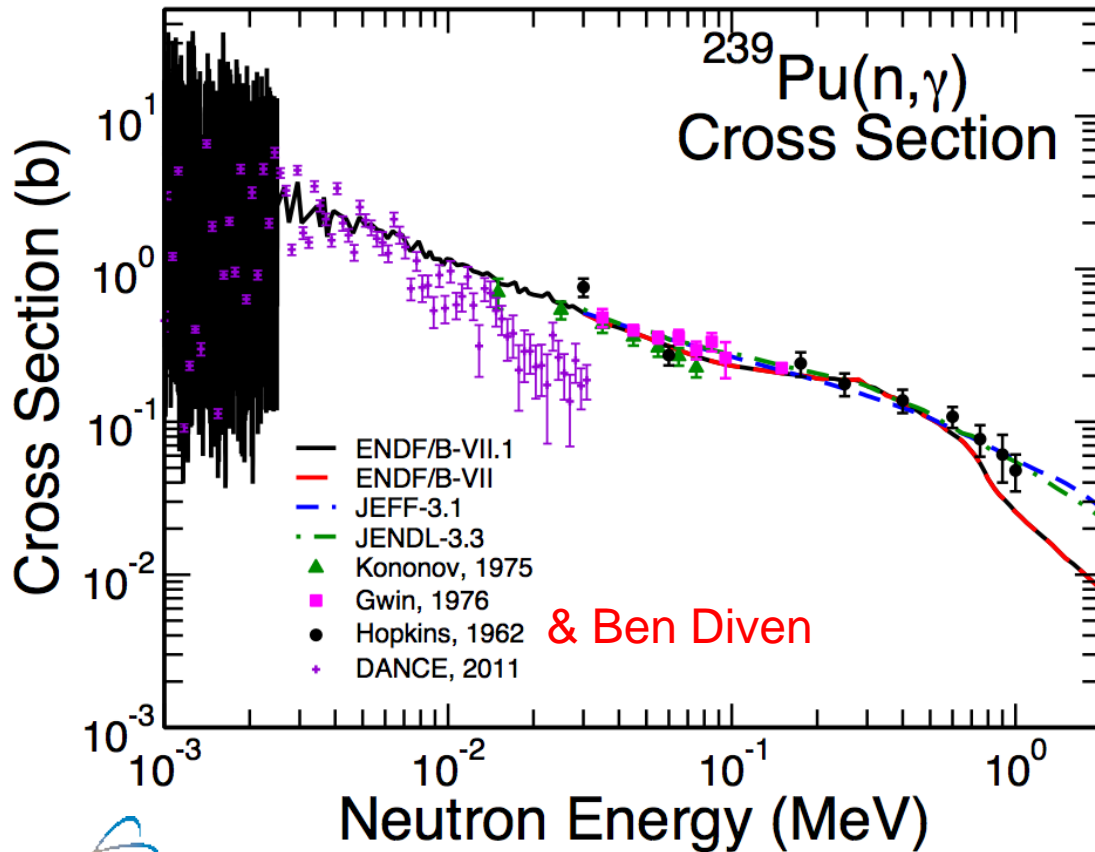
Black = snapshot of ongoing work. Will be updated to include Lestone, Chatillon, etc

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



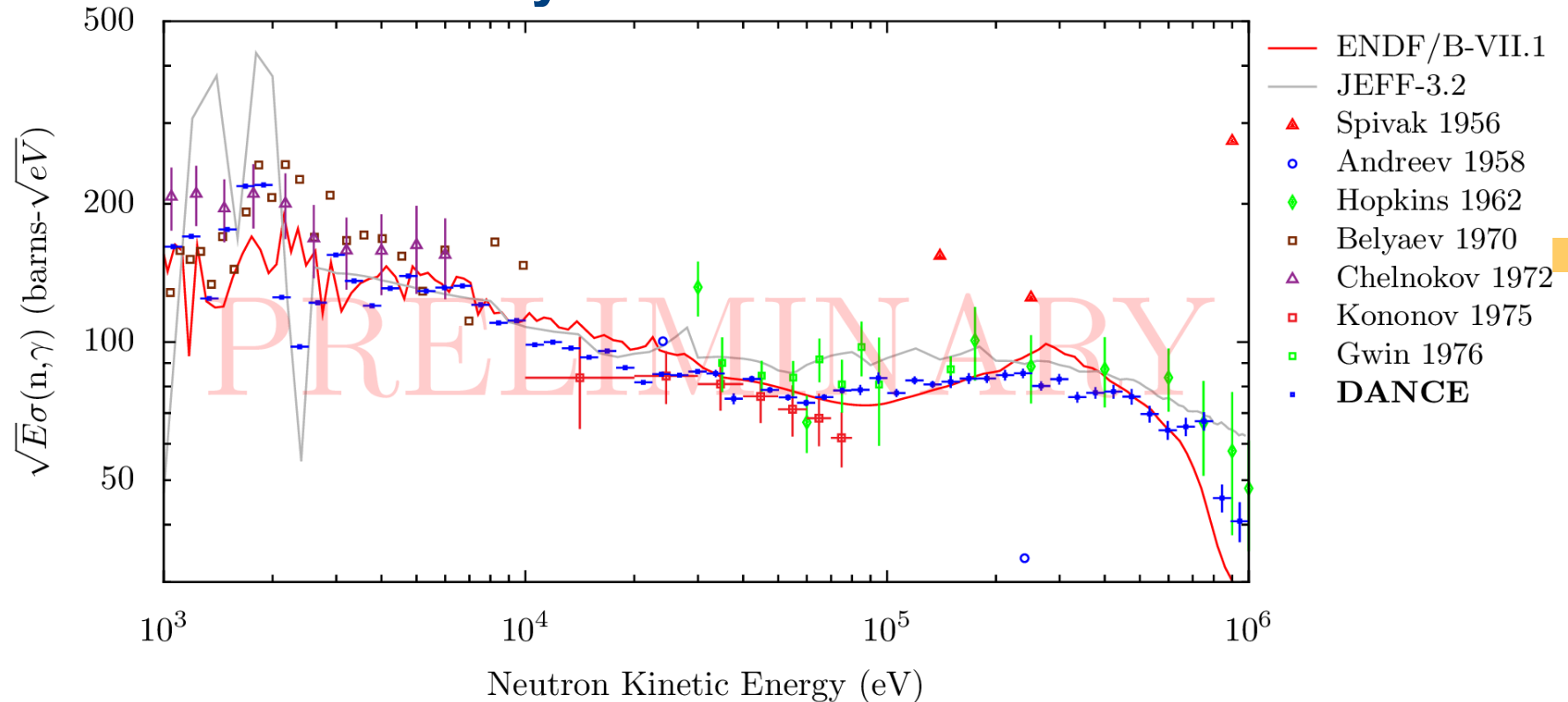
# Plutonium Capture: Improvements Are Needed

Existing uncertainties >15%



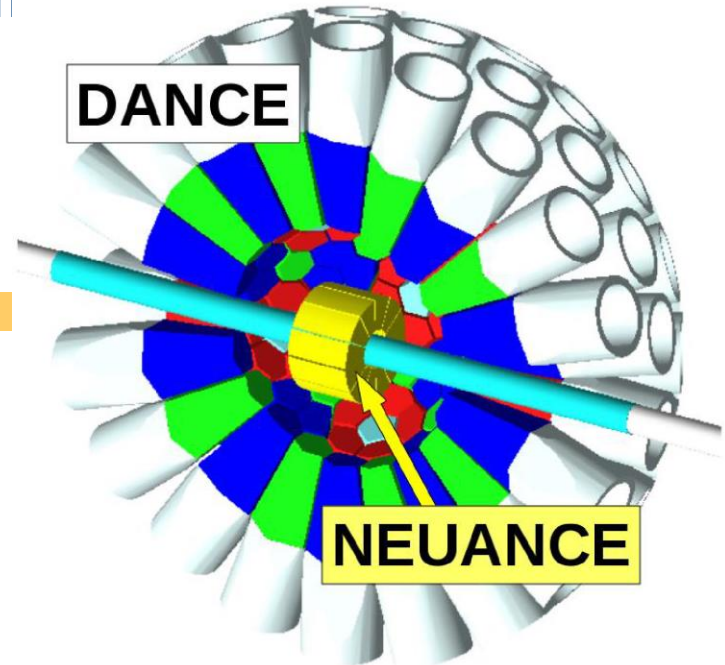
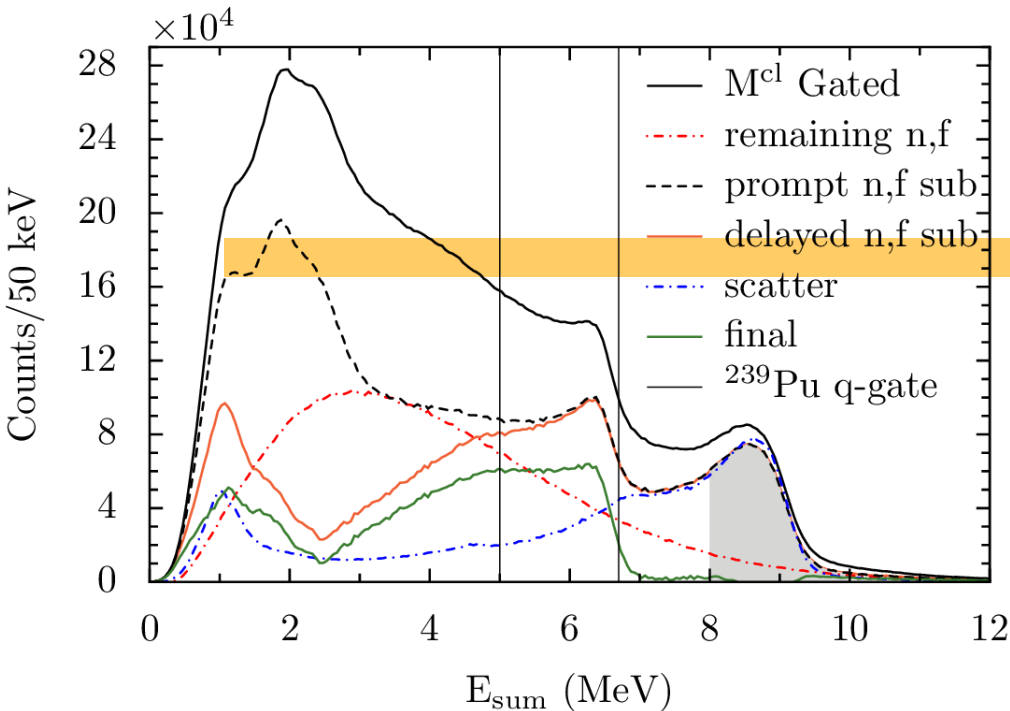
- ◆ SG33 & PROFIL (PHENIX)  $^{239}\text{Pu}(n,g)$  integral testing suggests B-VII is ~ 10% low over this fast reactor spectrum. Also, Ishikawa's ADJ work suggests JENDL should be raised 5-10%
- ◆ DANCE measurements now being analyzed

# 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

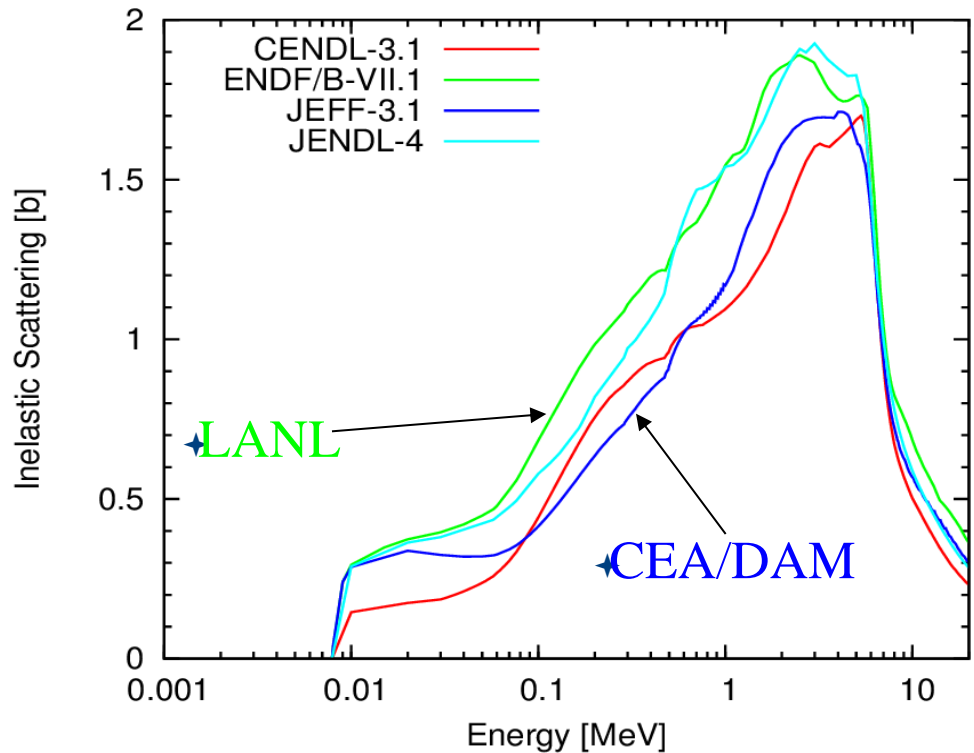
## IAEA Technical Meeting on Model Calculation for Major Actinides

- Summary report published: INDC(NDS)-0597, R. Capote, et al.

✦ These two files equally work for Jezebel keff prediction.

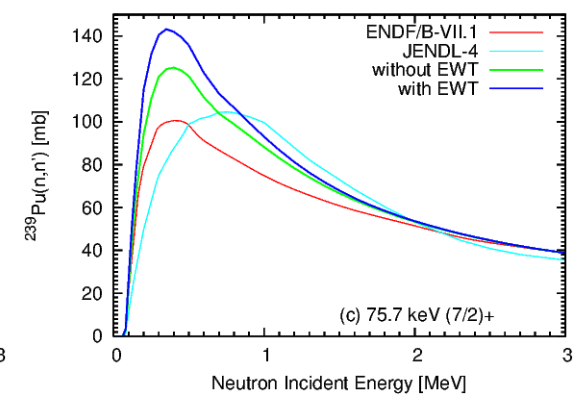
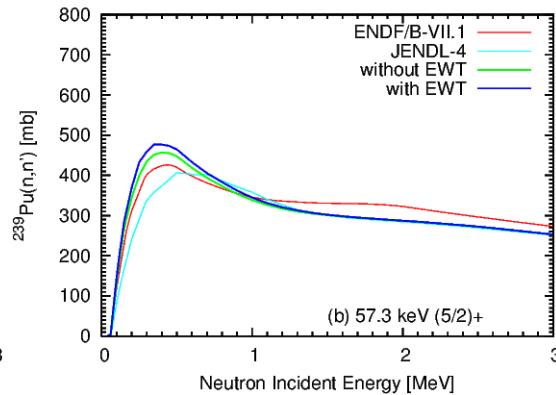
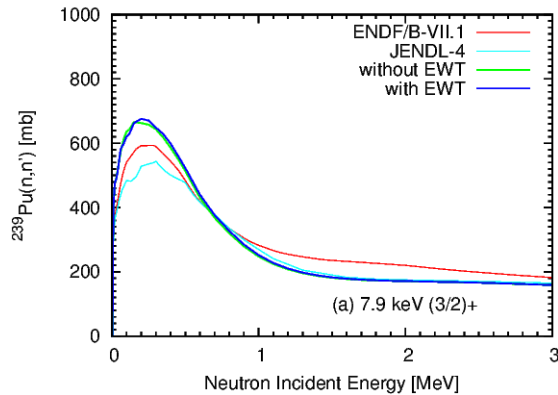
✦ Probably, the difference in the inelastic scattering comes from the optical potential parameters adopted in each library

- 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

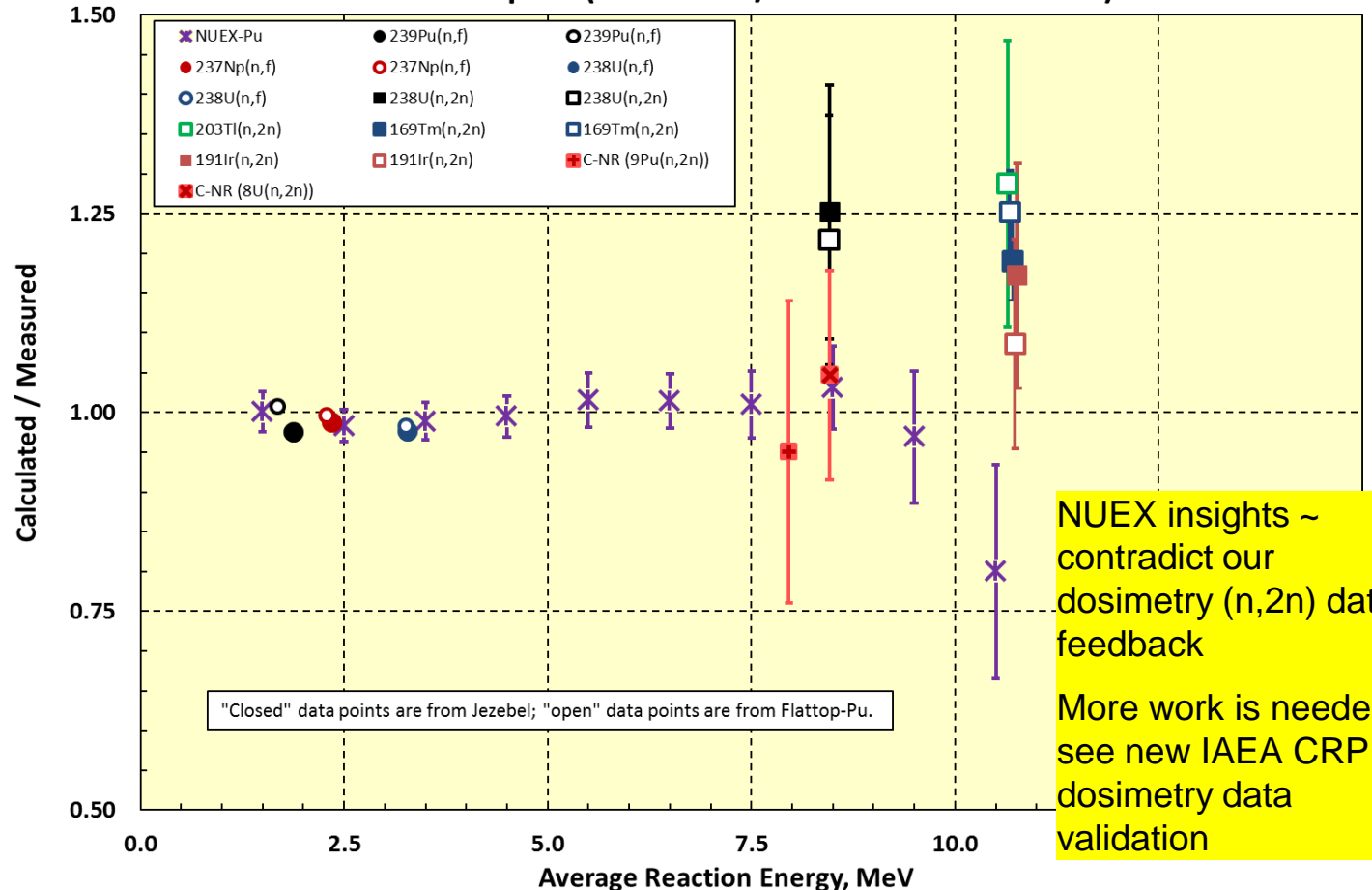


# Reaction Rates in Fast Critical Assemblies Provide Integral Test of Prompt Fission Neutron Spectrum & (n,2n) Cross Sections - *Plutonium-239 PFNS Data*

**<sup>239</sup>Pu**

**With NUEX  
data added  
(Lestone)**

Selected Spectral Index Data for the Central Region of Jezebel  
or Flattop-Pu (with ENDF/B-VII.1 Cross Sections)



# New $^{16}\text{O}$ Evaluation Based on R-Matrix Analysis of the $^{17}\text{O}$ System

G. M. Hale and M. W. Paris, T2

# Major advances for 16O

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- **Higher (n,a) cross sections informed by both Georginis re-analysis of older data, and by constraints from scattering theory**
- **Lower total/elastic low-energy cross section**
  - not quite as low as Kopecky-Plompen analysis, but lower than B-VII
- **Total cross section validated though recent RPI measurement**
  - Confirmation data, obtained after evaluation was completed, agrees to 1%

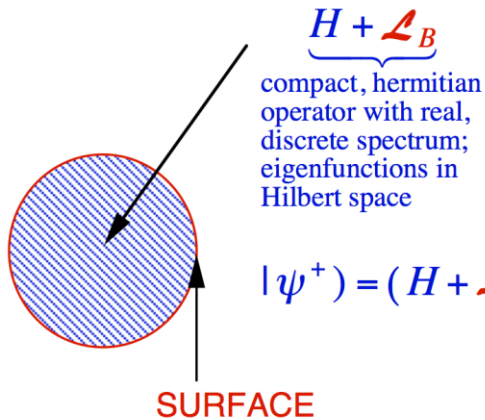
# Outline

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- **Reminder of R-matrix properties, EDA code**
- **Status of the  $^{17}\text{O}$  system analysis and  $^{16}\text{O}$  evaluation**
  - ⑩ **Low-energy scattering cross sections**
  - ⑩  **$^{13}\text{C}(\alpha, n)$  and  $^{16}\text{O}(n, \alpha_0)$  cross sections**
  - ⑩ **Fits, data renormalizations, etc.**
  - ⑩ **Extension of the evaluation to higher energies**
- **Summary and conclusions**

# R-matrix Formalism

INTERIOR (Many-Body) REGION  
(Microscopic Calculations)



$$\mathcal{L}_B = \sum_c |c\rangle \left( d \left( \frac{\partial}{\partial r_c} r_c - B_c \right) \right)$$

$$\langle \mathbf{r}_c | c \rangle = \frac{\hbar}{\sqrt{2\mu_c a_c}} \frac{\delta(r_c - a_c)}{r_c} \left[ (\phi_{s_1}^{\mu_1} \otimes \phi_{s_2}^{\mu_2})_s^\mu \otimes Y_l^m(\hat{\mathbf{r}}_c) \right]_J^M$$

$$R_{c'c} = \langle c' | (H + \mathcal{L}_B - E)^{-1} | c \rangle = \sum_\lambda \frac{\langle c' | \lambda \rangle \langle \lambda | c \rangle}{E_\lambda - E}$$

ASYMPTOTIC REGION  
(S-matrix, phase shifts, etc.)

$$\langle r_{c'} | \psi_c^+ \rangle = -I_{c'}(r_{c'}) \delta_{c'c} + O_{c'}(r_{c'}) S_{c'c}$$

or equivalently,

$$\langle r_{c'} | \psi_c^+ \rangle = F_{c'}(r_{c'}) \delta_{c'c} + O_{c'}(r_{c'}) T_{c'c}$$

Measurements

# R-Matrix Analysis of Reactions in the $^{17}\text{O}$ System

channel	$a_c$ (fm)	$l_{\max}$
$n+^{16}\text{O}$	4.4	4
$\alpha+^{13}\text{C}$	5.4	5

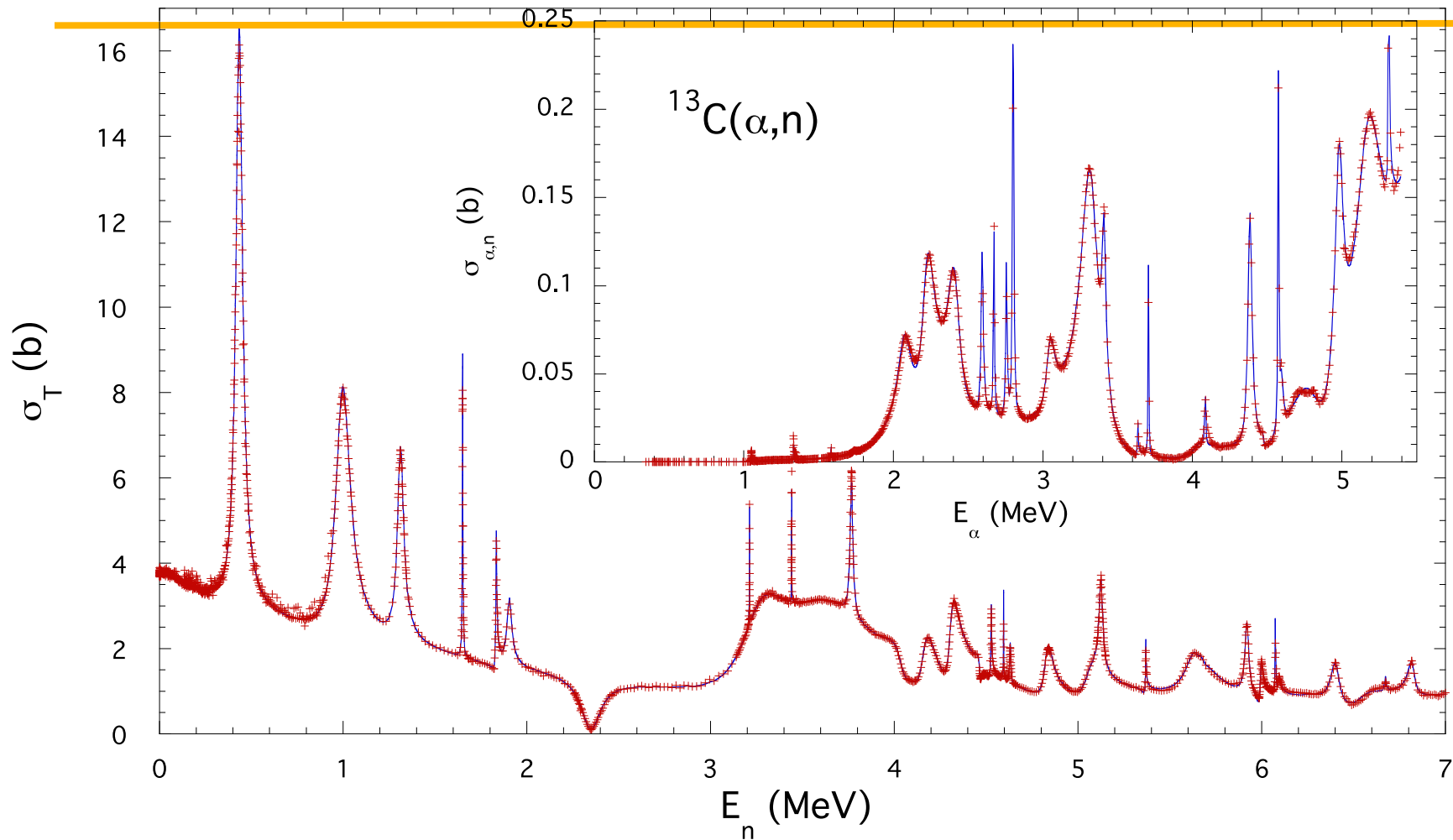
Reaction	Energies (MeV)	# data points	Data types
$^{16}\text{O}(n,n)^{16}\text{O}$	$E_n = 0 - 7$	2540	$\sigma_T, \sigma(\theta), P_n(\theta)$
$^{16}\text{O}(n,\alpha)^{13}\text{C}$	$E_n = 2.35 - 5$	672	$\sigma_{\text{int}}, \sigma(\theta), A_n(\theta)$
$^{13}\text{C}(\alpha,n)^{16}\text{O}$	$E_\alpha = 0 - 5.4$	870	$\sigma_{\text{int}}$
$^{13}\text{C}(\alpha,\alpha)^{13}\text{C}$	$E_\alpha = 2 - 5.7$	1168	$\sigma(\theta)$
total		5250	8

$\chi^2$  per degree of freedom = 1.68

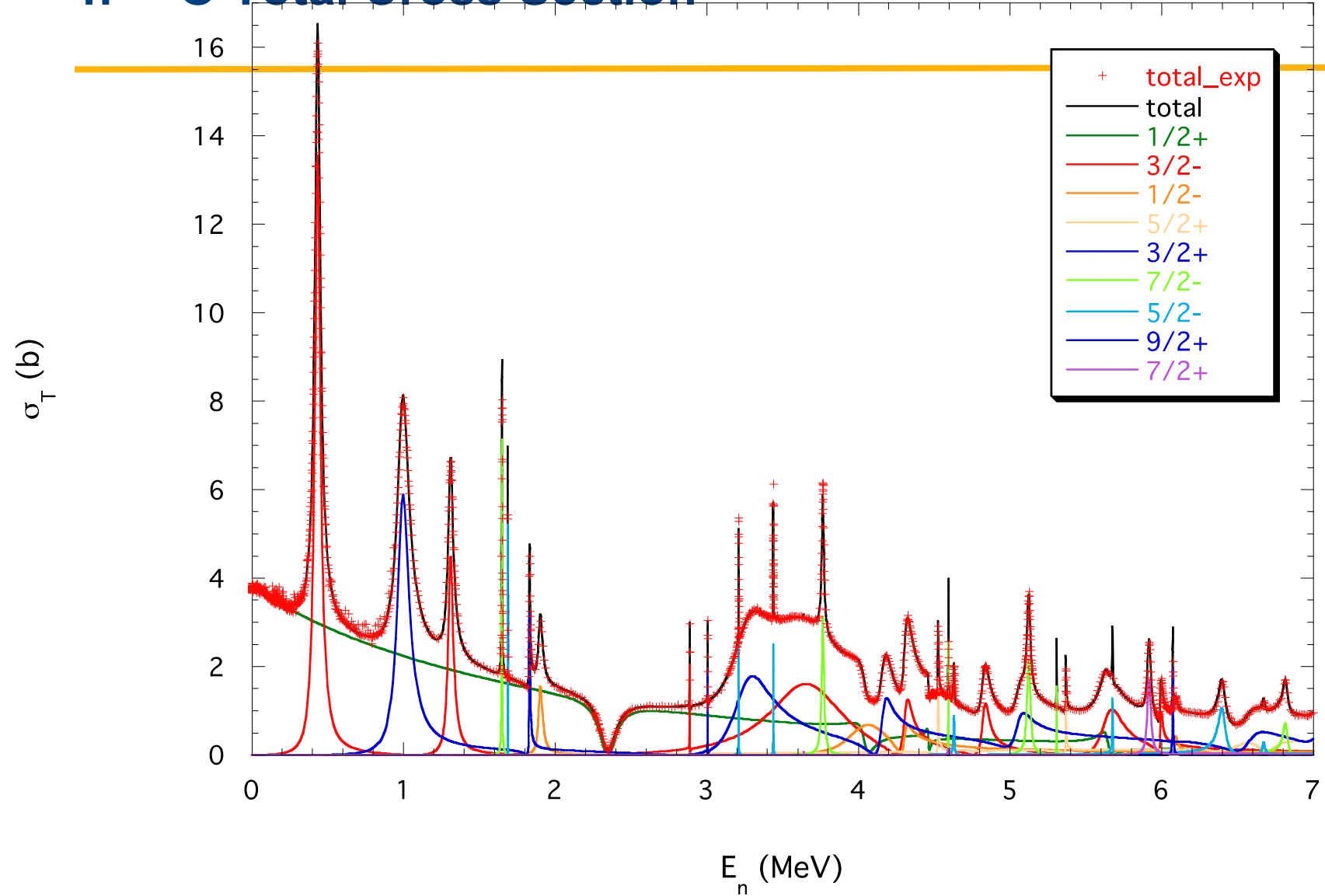
## Total Cross Section Data

✦Authors (n,n):	✦Energy Range	✦Energy Shift	✦Normalization
✦Schneider	✦0.0253 eV	✦0	✦1.0 (fixed)
✦Dilg, Koester, Block	✦0.13 – 23.5 keV	✦0	✦1.0 (fixed)
✦Ohkubo (corr. for H)	✦0.8 – 935 keV	✦0	✦0.9989
✦Johnson &	✦49 – 3139 keV	✦0	✦0.9799
✦Authors ( $\alpha$ ,n):	✦Energy Range	✦Energy Shift	✦Normalization
✦Drotleff et al.	✦346 – 1389 keV	✦0	✦1.0 (fixed)
✦Heil et al.	✦416–899 keV	✦0	✦1.0 (fixed)
✦Kellogg	✦445–1045 keV	✦0	✦1.506
✦Bair and Haas	✦0.997–5.402 MeV	✦4 keV	✦0.9410

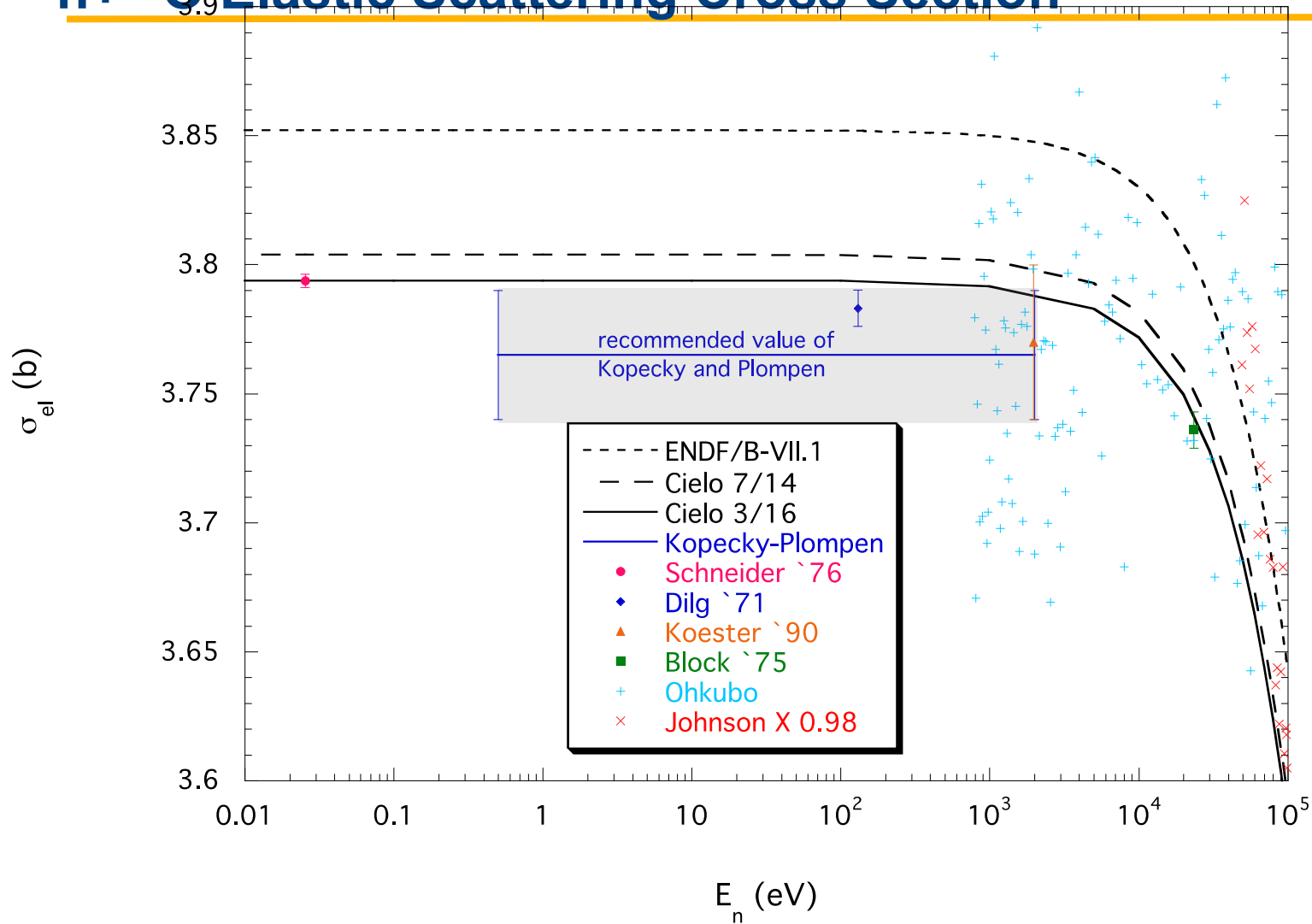
# Integrated (total) Cross Sections



# $n+^{16}\text{O}$ Total Cross Section



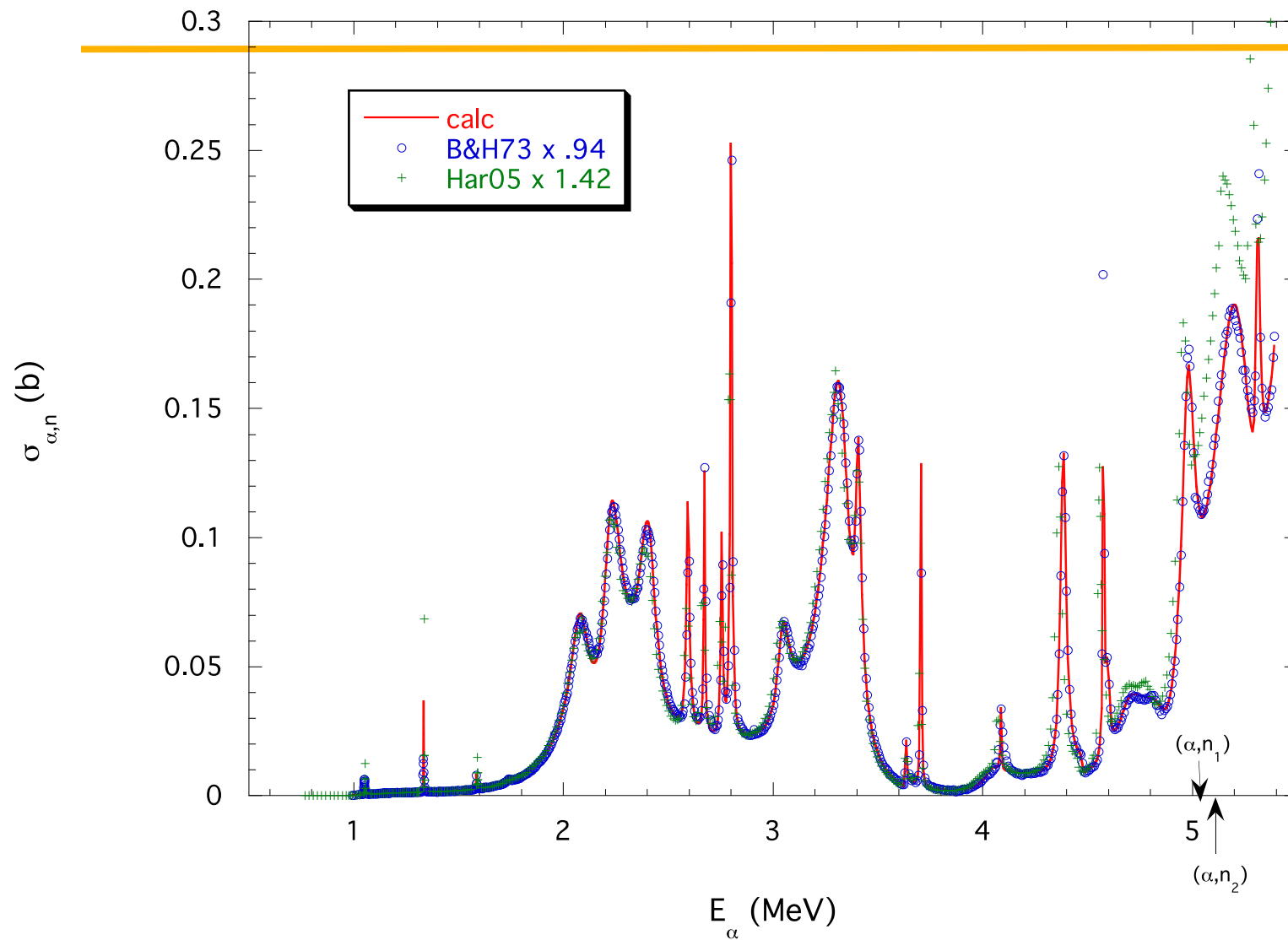
# $n+^{16}\text{O}$ Elastic Scattering Cross Section



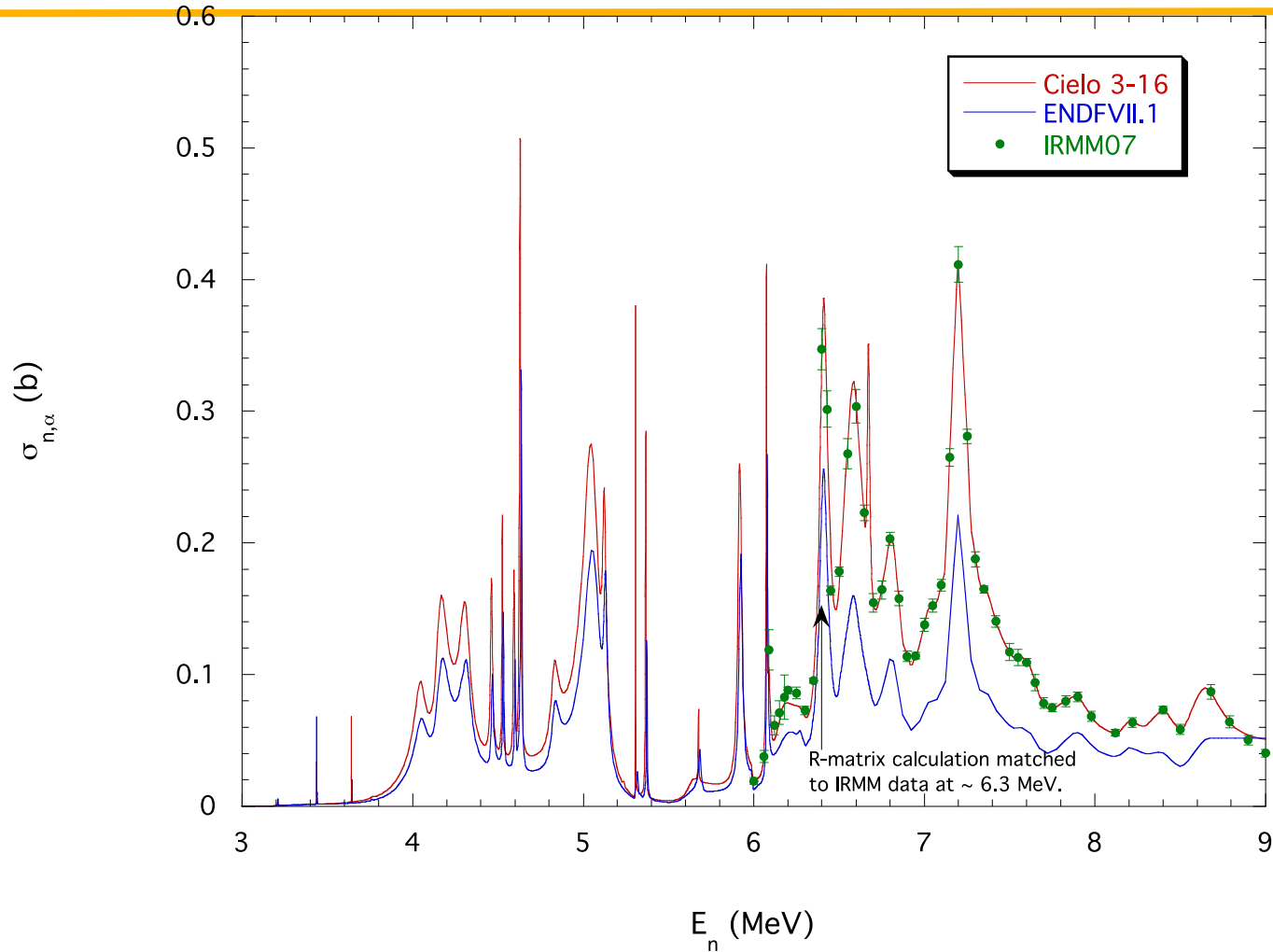
## Giorginis' Analysis of ( $\alpha$ ,n) Measurements

- Considered two measurements, Bair and Haas (B&H73) and Harissopoulos *et al.* (Har05).
- Determined a preliminary cross-section scale for B&H73 based on the integral of the thick-target yield over the narrow resonance at 1.056 MeV that agrees with the published scale of Har05.
- Then applied a correction common to both data sets related to characterization of the  $^{13}\text{C}$  target that gives the cross-section scales **0.95×B&H73** and **~1.42×Har05**.
- Considers the relative shape of the B&H73 measurement to be the most accurate since it had the thinnest target.

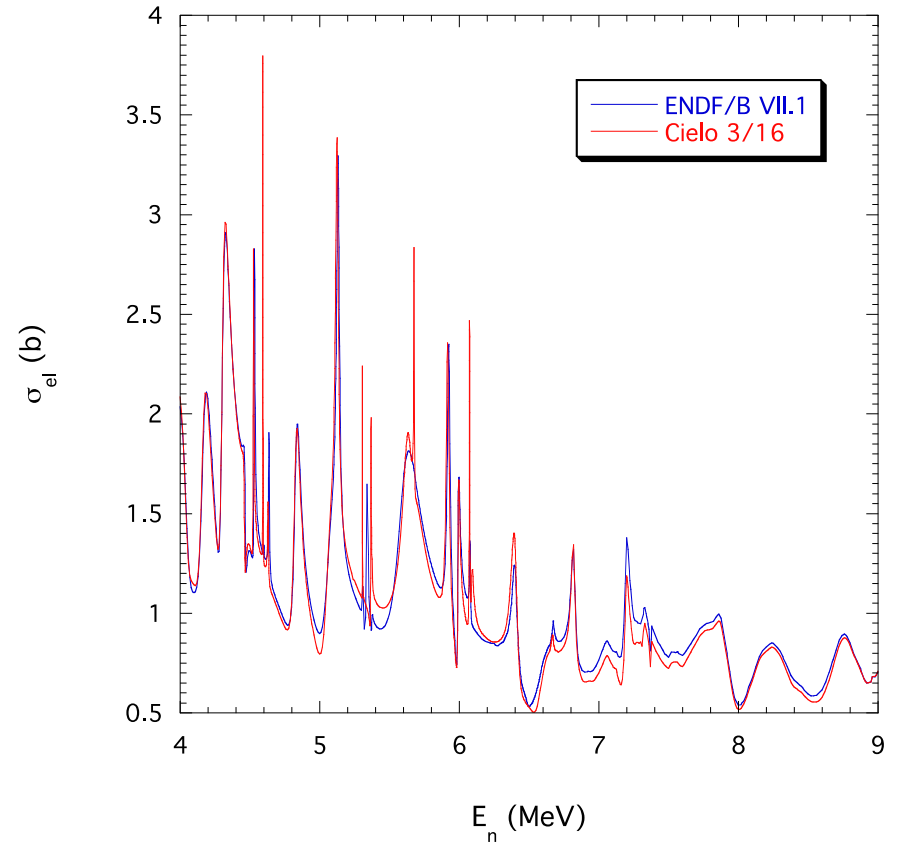
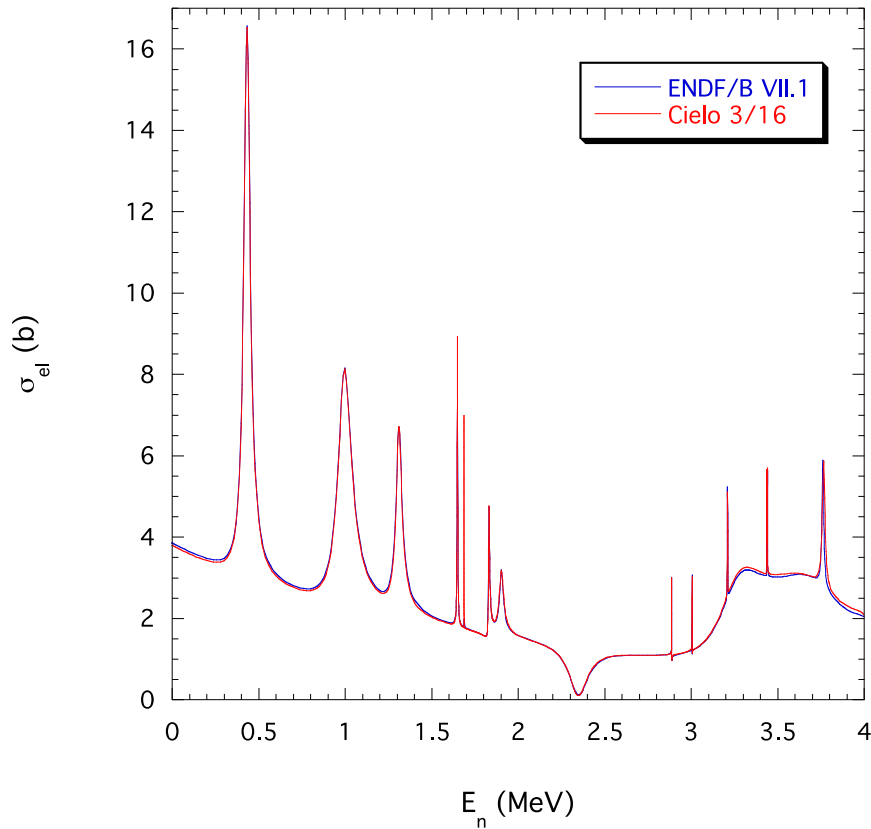
# $^{13}\text{C}(\alpha, n)^{16}\text{O}$ Cross Section



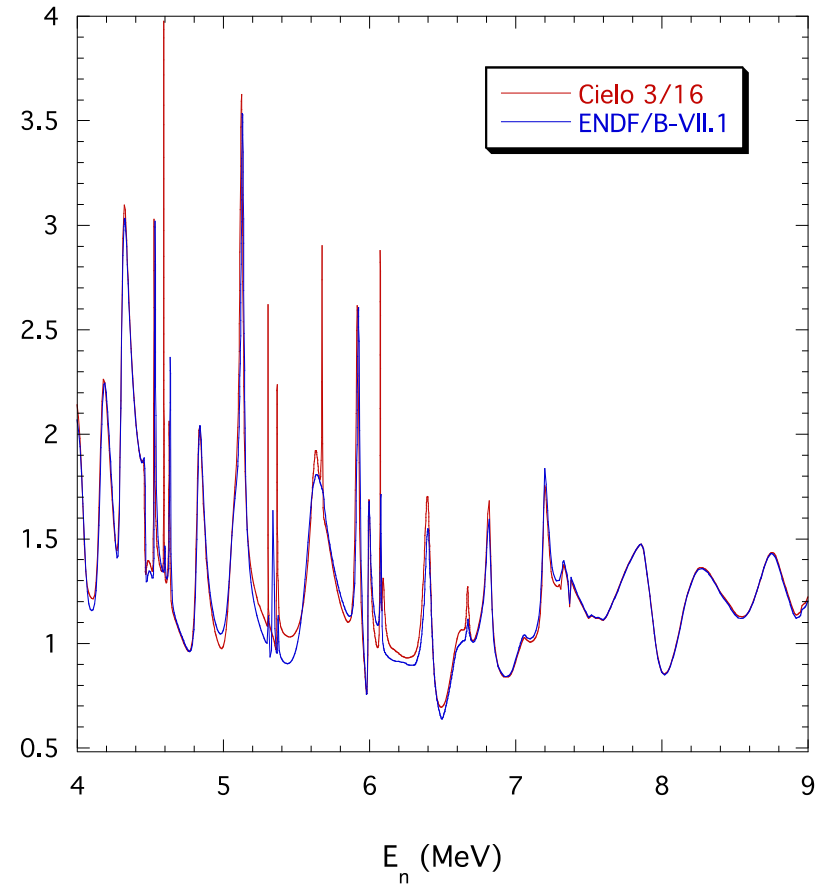
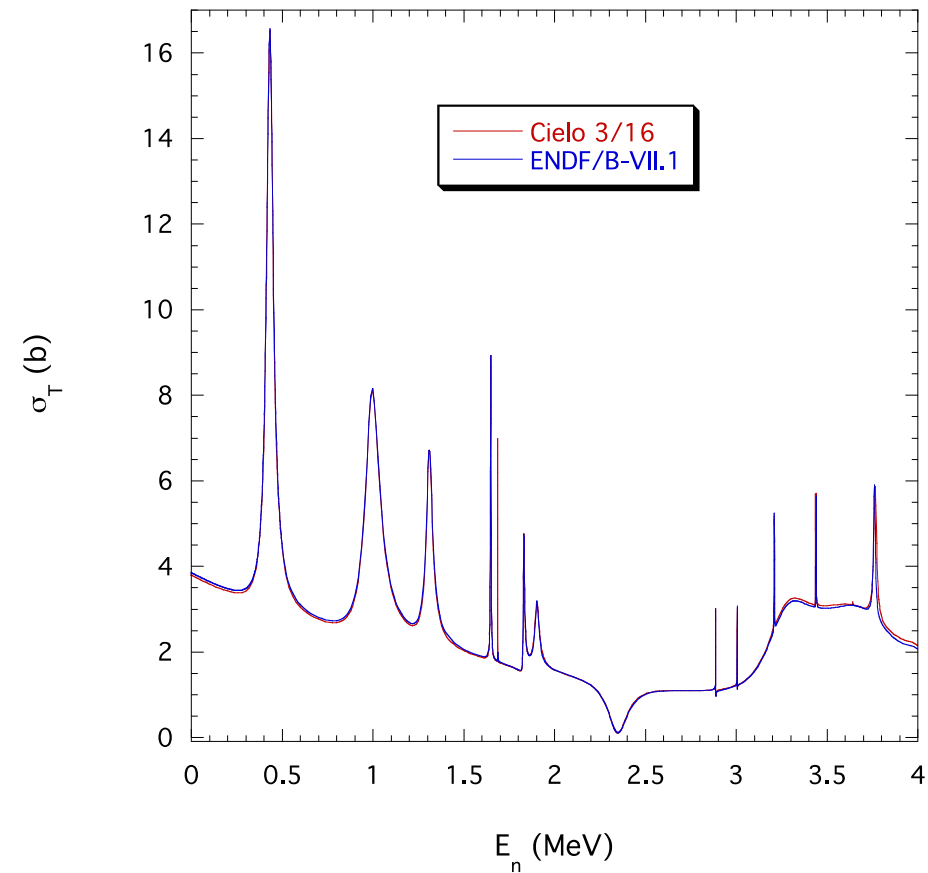
# $^{16}\text{O}(n,\alpha_0)^{13}\text{C}$ Cross Section



# n+<sup>16</sup>O Elastic Cross Section

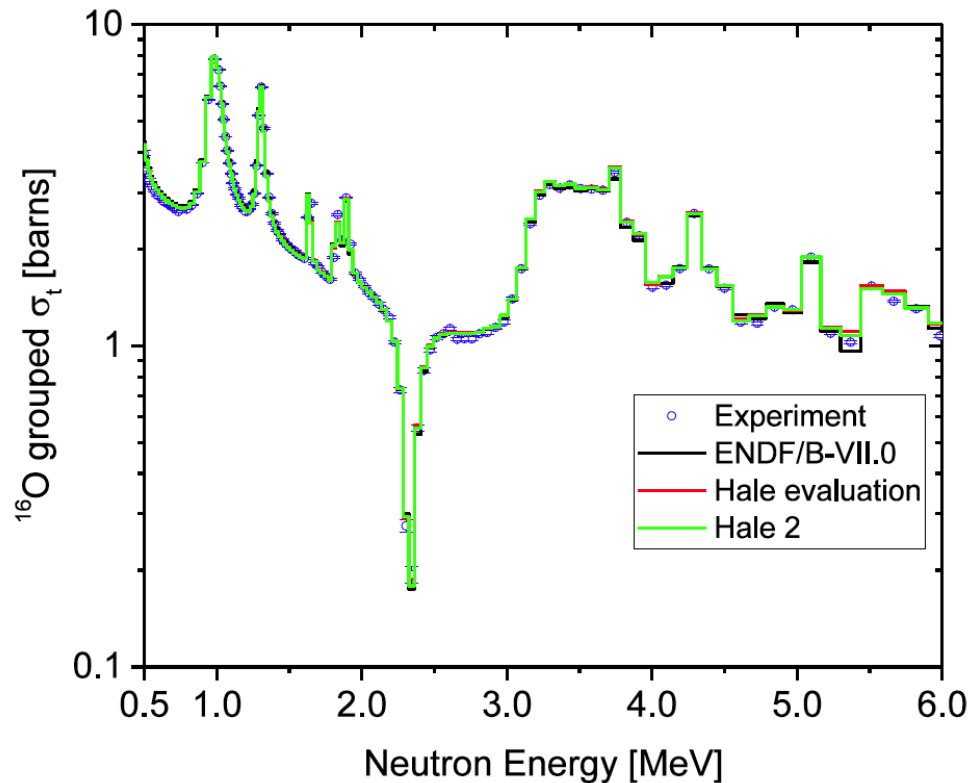


# $n+^{16}\text{O}$ Total Cross Section



# $n+^{16}\text{O}$ Total Cross Section – Comparison to RPI: Integral in 3.2-6 MeV region, $C/E=1.005 \pm 0.003$ . (Confirmatory data, not included in Hale's analysis),

## Grouped Cross Section



Hale estimate of his evaluated uncertainties:

0.5 - 2.0 MeV: 1.99 %

2.0 - 3.2 MeV: 3.03 %

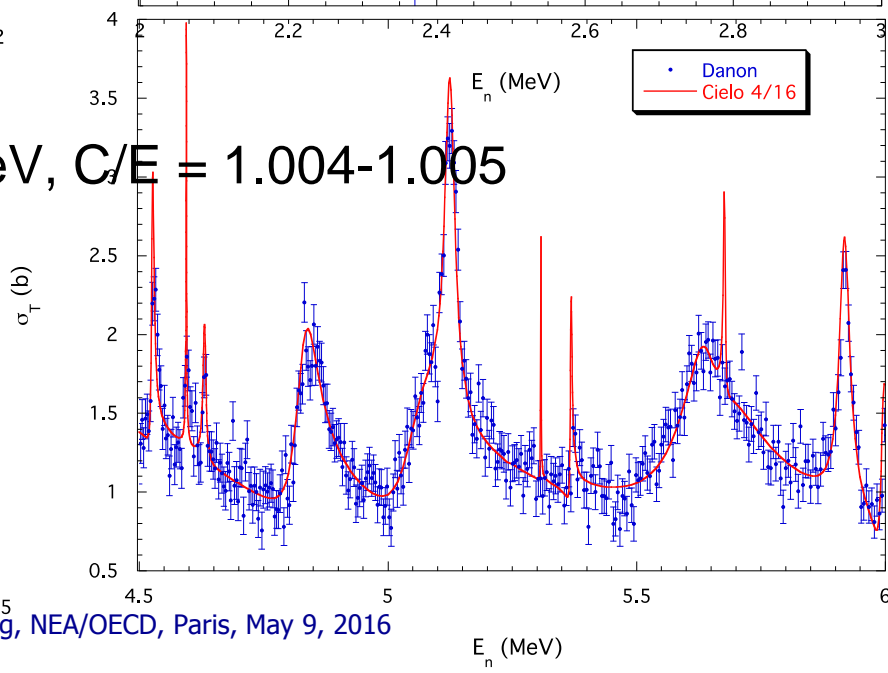
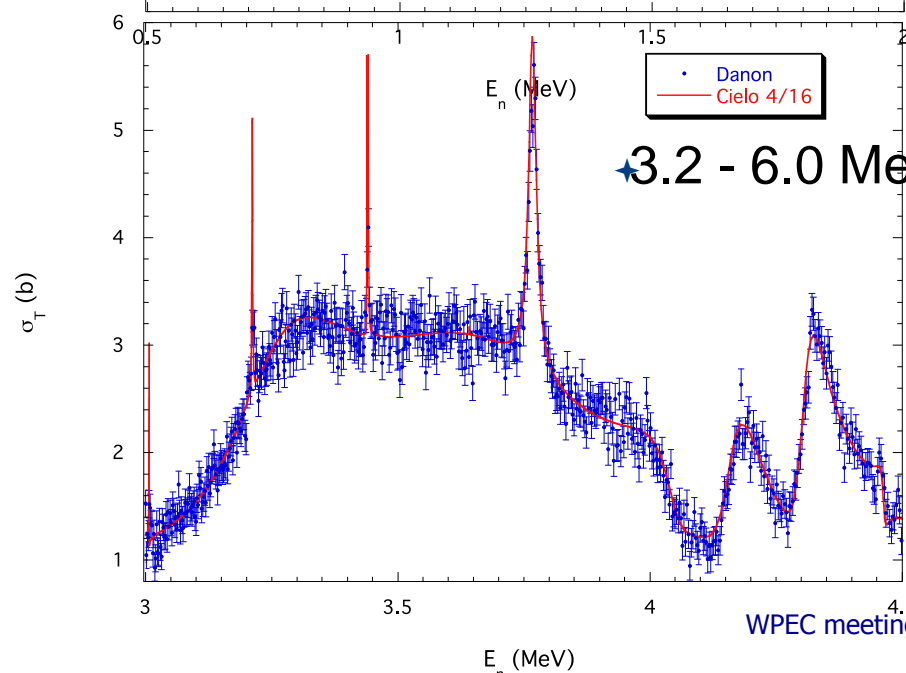
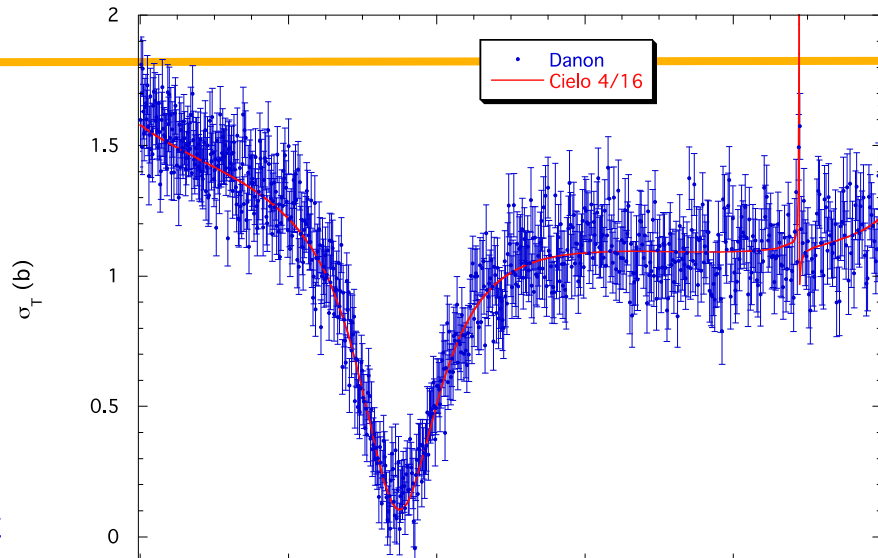
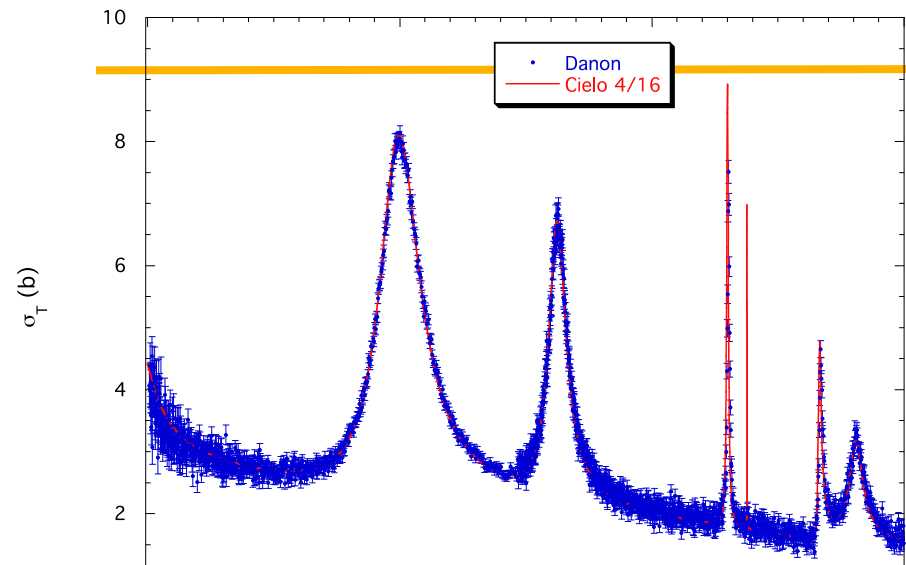
3.2 - 6.0 MeV: 2.60 %

6.0 - 9.0 MeV: 7.59 %

# Comparison to RPI Total Cross Section - Data after evaluation

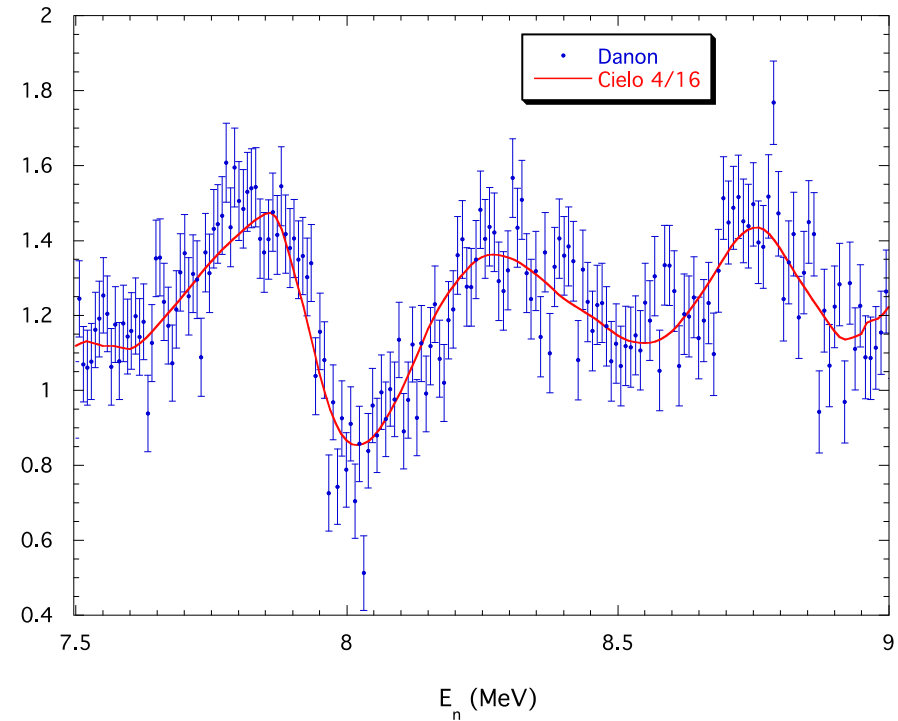
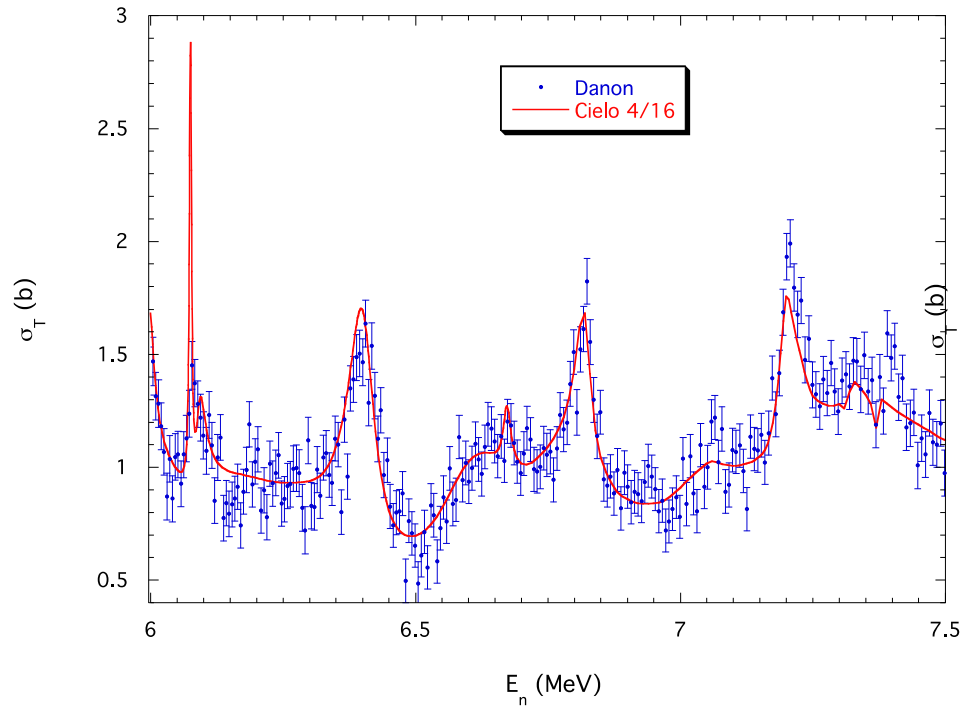
0.5 - 2.0 MeV, C/E = 0.996

2.0 - 3.2 MeV, C/E = 0.988-0.990

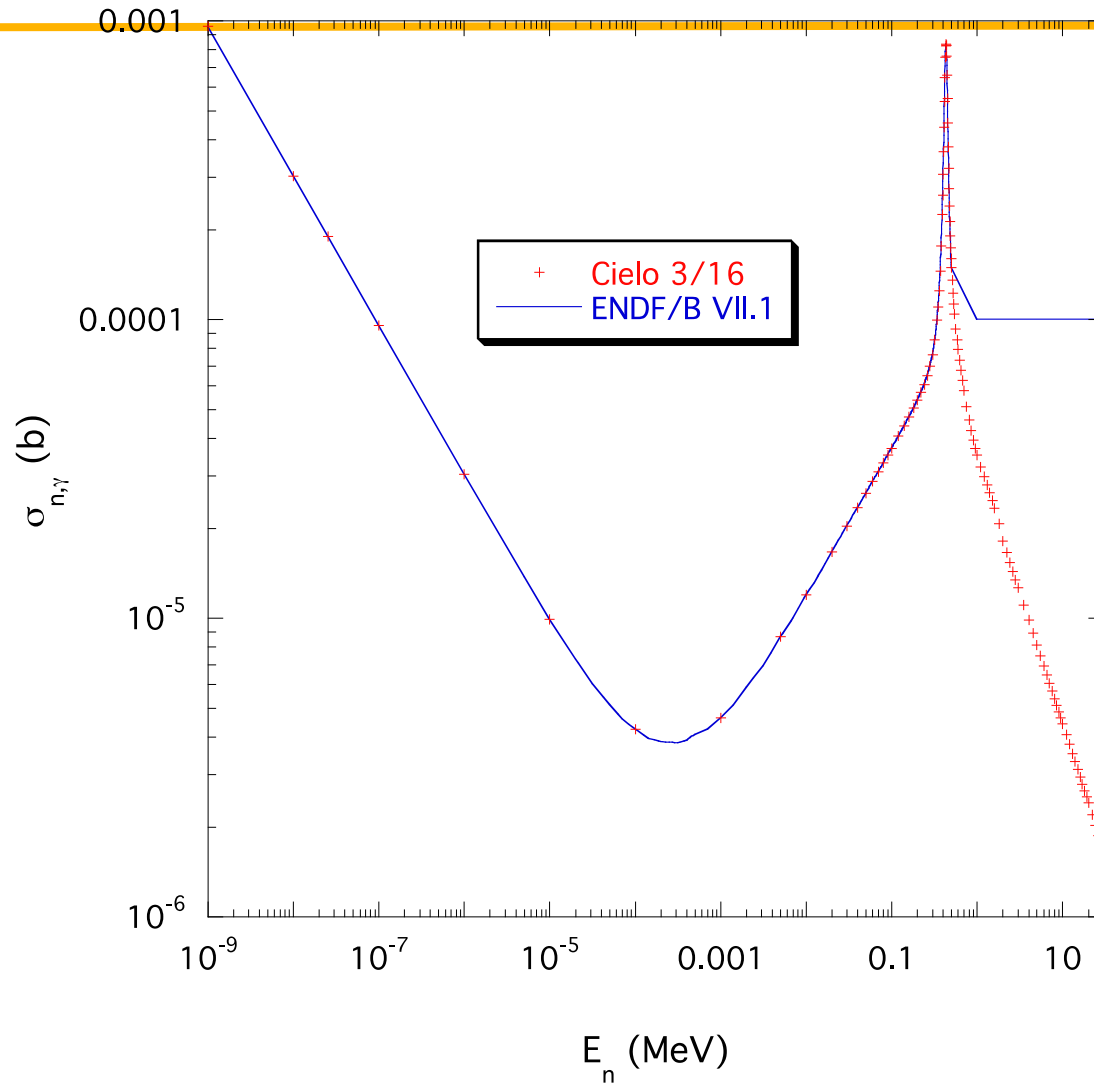


# Comparison, cont.

6.0 - 9.0 MeV, C/E = 0.992



# Capture Cross Section



# Summary and Conclusions

---

- **R-matrix descriptions are constrained by fundamental properties (unitarity, causality, TRI) of nuclear reaction theory.**
- **EDA analysis of the  $^{17}\text{O}$  system includes data from all possible reactions, giving results that are highly constrained by the properties above (especially unitarity).**
- **The low-energy  $n+^{16}\text{O}$  scattering cross sections are now in better agreement with high-precision measurements, and the  $(n,\alpha_0)$  cross section agrees with the data of B&H73, IRMM07 (Giorginis).**
- **The evaluated  $^{16}\text{O}$  file Cielo 3/16 extends to 150 MeV, and is the same as ENDF/B VII.1 above 9 MeV (except for capture).**

## 56Fe iron evaluation advances - BNL, IAEA, ORNL, IRNS

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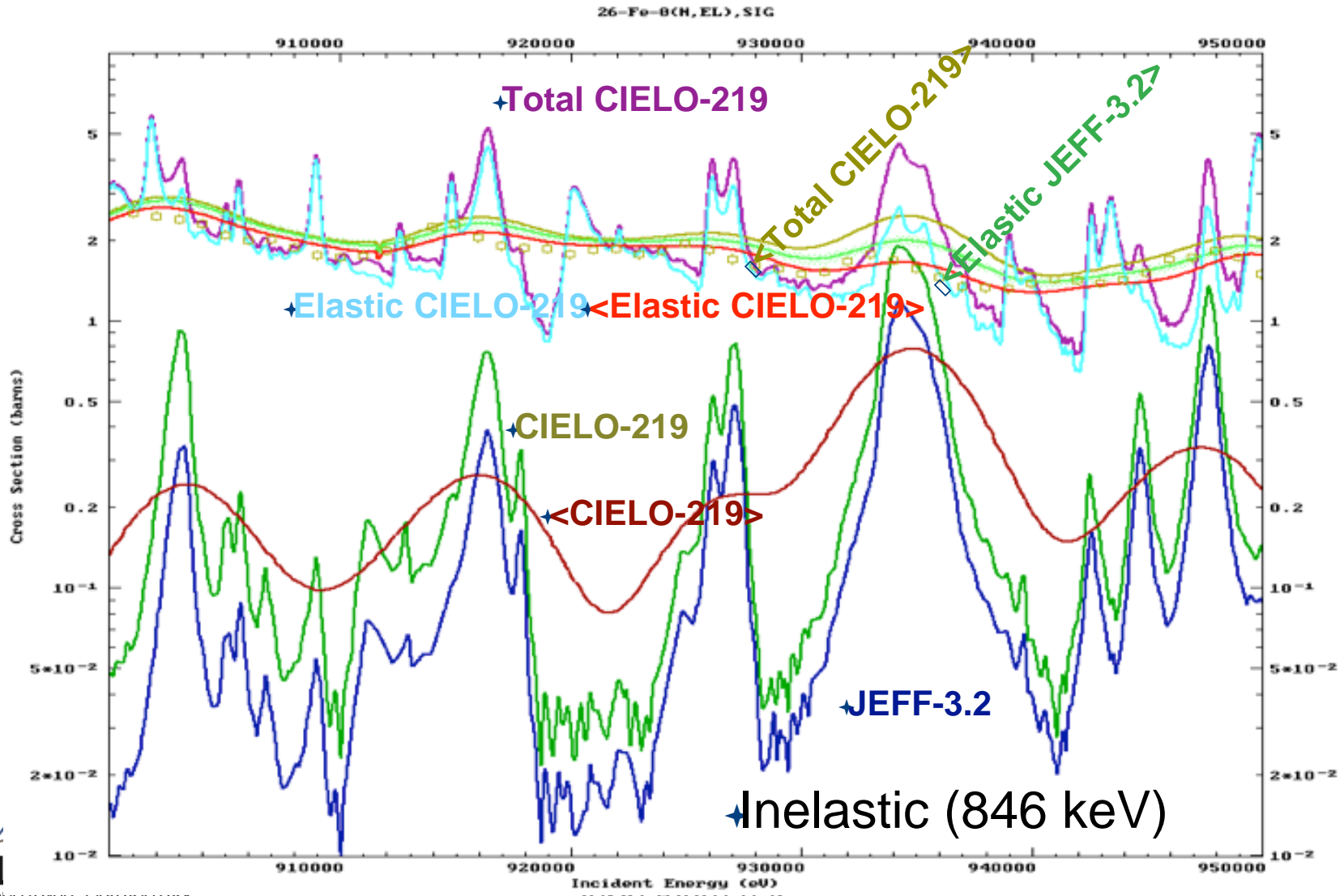
- New evaluation makes use of most precise and most recent experimental data between resonance region and 4 MeV (Berthold data for total, new Geel (Negret, Plompen) data for inelastic, and old but not used before data by Dupont for inelastic, Kinney data for elastic angular distributions)
- It uses IRDFF file for the dosimetry reaction (n,p) (calculations agree with IRDFF within uncertainties except of low incident energies)
- Employs dispersive, Lane-consistent optical model above 4 MeV
- Uses consistent modeling up to 150 MeV
- Is informed by the semi-integral data from RPI (neutron emission and capture)
- Provides better reproduction of inelastic (low energies by construction, higher energies by improved modeling)

# 56Fe iron evaluation advances - BNL, IAEA, ORNL, IRNS

---

- Reproduces experimental neutron spectra better than in VII.1
- Improves agreement for the criticality benchmarks by adjusting angular distributions in the resonance region and adding background to capture to simulate the effect of lost d-wave resonances (we'll work on resonance region to remove backgrounds and angular distribution tweaks while maintain benchmark results)

# nat-Fe: Total, Elastic, Inelastic 900-950 keV



# Elastic angular distributions

**Kinney data are the most extensive and detailed above the inelastic threshold**

**JEF-2.2=>JEFF-3.2 ang. distr. are fitted to the Kinney data**

**Whenever low energy-resolution experimental data are available they are closer to EMPIRE than to Kinney**

**However, RPI semi-integral experiment favors JEF(F)s so we adopted it between 846 keV and 4 MeV**

**RPI broad-average data compared with EMPIRE and broad-averaged**

**Evaluations**

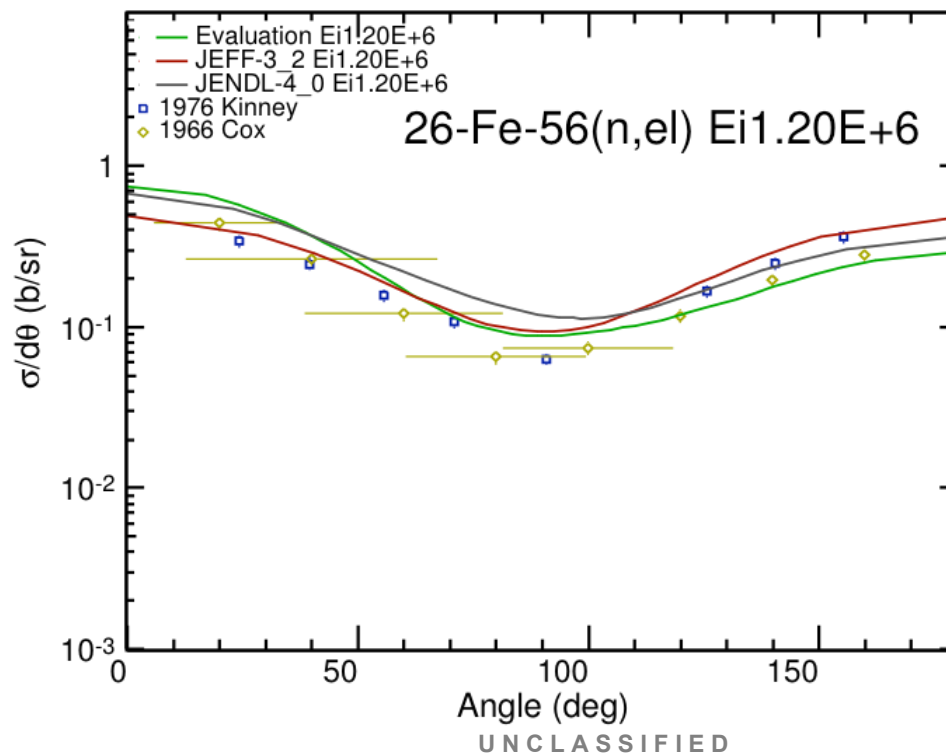
NATIONAL LABORATORY

EST. 1943

UNCLASSIFIED

# Elastic angular distributions – Kinney data

★ CIELO-219



★ EMPIRE

# 235U iron evaluation advances - IAEA, ORNL, IRNS, LANL & Performance in Criticality Simulations – Low energy RR

---

- fit of Thermal Neutron Constants (TNC) based on microscopic experiments results in a higher thermal fission ( $\sim 587$  barns) and capture ( $\sim 100$  barns) cross sections, and lower total nubar (2.4216 vs 2.4368)
- new resonance parameters fitted to the new TNC and resonance integrals recommended by the Neutron Standard committee, and tuned on integral data
- new evaluation of PFNS that agrees well with microscopic measurements and corresponds to a lower  $^{235}\text{U}$  thermal PFNS average energy (now 2.00 MeV, before - 2.03 MeV) that increases criticality

## 235U iron evaluation advances - IAEA, ORNL, IRNS, LANL & *Performance in Criticality Simulations – Low energy*

---

- the higher  $^{16}\text{O}$  cross sections leads to more neutron absorption and reduces criticality of epithermal assemblies
- new TSL on hydrogen slightly increases criticality of thermal solutions
- strong energy dependence of resonance nubar based on measured data from 0.3 eV up to 60 eV reduces criticality of epithermal assemblies
- decrease of neutron capture around 1 keV and above that increases criticality for intermediate assemblies (still to be compensated)

# 235U iron evaluation advances - IAEA, ORNL, IRNS, LANL & Performance in Criticality Simulations – Fast energies

---

- Optical model for fission describes Neutron Standard fission cross sections on U-235 and U-238 within 3% using double and triple humped barriers with absorption. Such accuracy allows for a better prediction of elastic and inelastic neutron scattering
- Interference of direct and compound mechanisms leads to the increase of inelastic cross sections from ~50 up to 500 keV on U-238
- Neutron scattering to collective states in the continuum is important to describe observed neutron emission spectra for incident neutron energies above 1 MeV
- increased inelastic scattering on U-238 above 500 keV up to 2 MeV, slightly decreased below.

## CIELO progress:

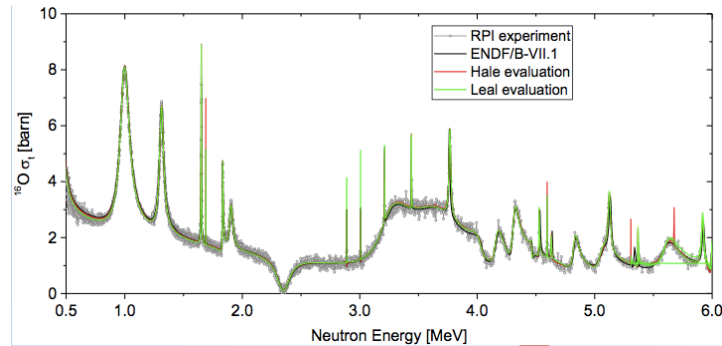
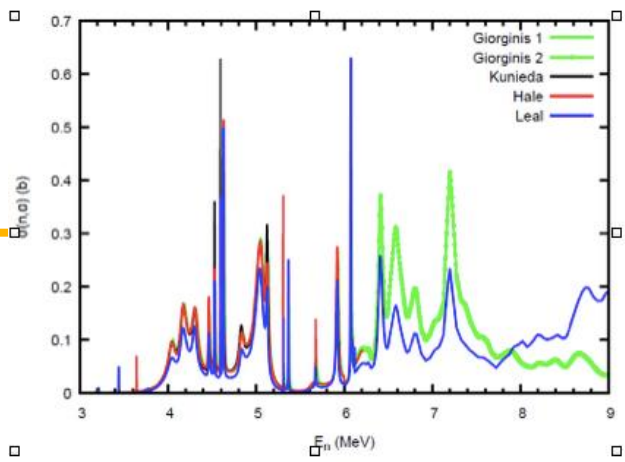
### (1) Resonance Region, extended to higher energies

---

Leal, Schillebeeckx, Noguerra, ... have made significant advances in representing our understanding of

- **235U** resonances, notably (n,g) near 1 keV, based on recent consistent data between RPI and LANSCE/DANCE
  - updates may be needed in 10s of KeV region too
- **238U** Geel measurements, which are leading to a new evaluation that is only a small perturbation compared to previous ENDF. Up to 20 keV.
  - The new (n,g) is leading to an update to the standards (similar result)
- **239Pu** resonances from SG34
- **56Fe** resonances up to 2 MeV with more rigorous angular distribution treatment

# CIELO progress: (2) 16O



Various files for testing, including R-matrix analyses from Hale and from Leal

- it appears that acceptable integral performance may be maintainable, following small updates to 235U nubar, and thermal PFNS

Questions remain on the magnitude of 16O(n, alpha), with discrepancies of order 30-50%, which have ~ 100 cpm impacts on criticality.

- new measurement is planned at LANL, in Fall-2015

Low-energy thermal elastic/total - consensus reached (3.765 barns)

A new total cross section has been obtained in the few-MeV region from RPI: “Game changer” (Lubitz).

3.2 MeV < E < 6 MeV	C/E	C/E Statistics
ENDF/B-VII.1	0.988	±0.002
Leal 1	1.030	±0.002
Leal 2	1.006	±0.002
Hale	1.012	±0.002
Cierjacks 80	0.968	±0.002

Normalization uncertainty:

$$\frac{\sigma_{\text{exp}}^H}{\sigma_{\text{ENDF}}^H} = 0.996 \pm 0.003^*$$

\*Statistical

## CIELO progress:

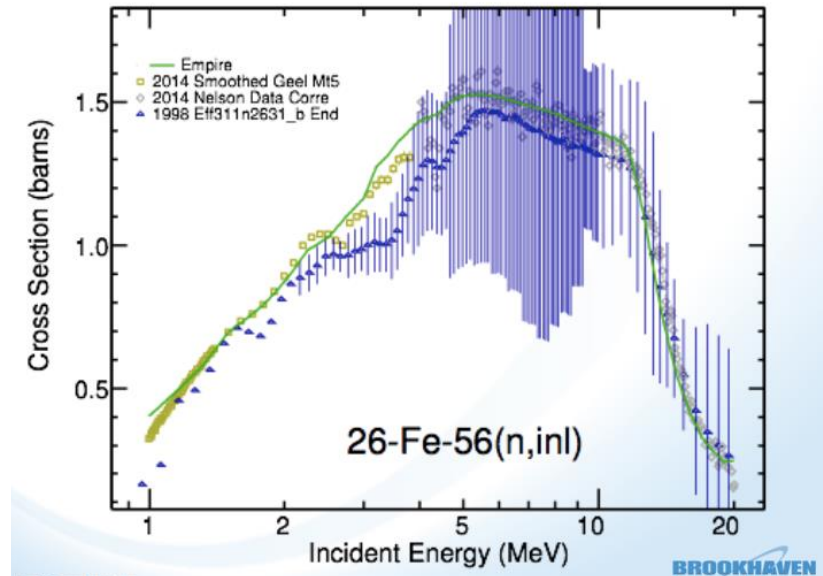
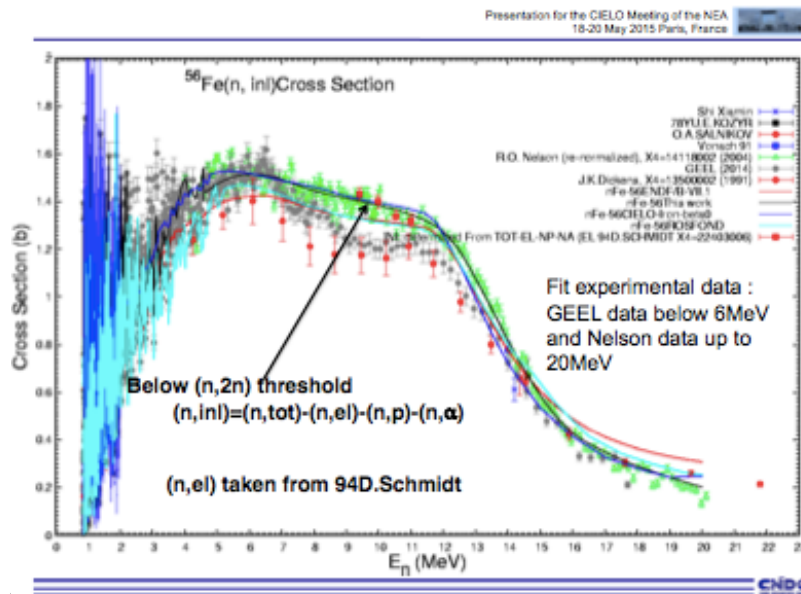
### (3) $^{56}\text{Fe}$ - using advanced EMPIRE modeling, & SAMMY to 2 MeV

New  $^{56}\text{Fe}$  evaluation produced as a “starter file”, BNL, IAEA, ... taking into account recent data from Geel & LANSCE on inelastic scattering, & RPI

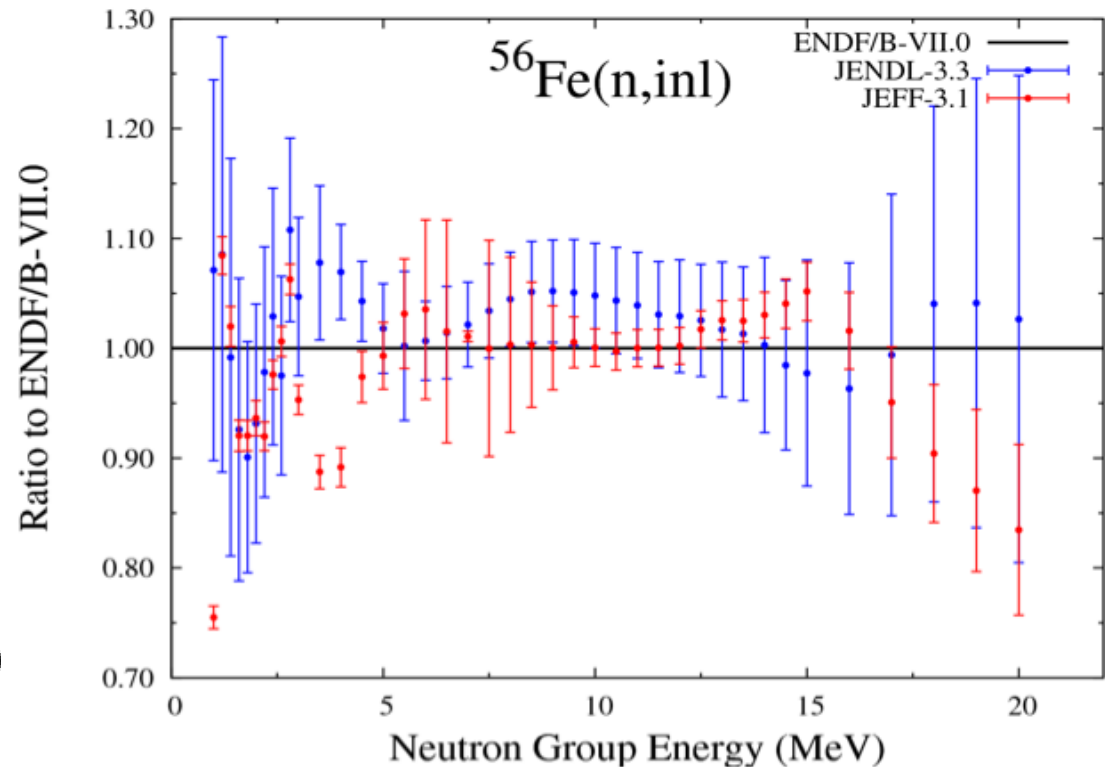
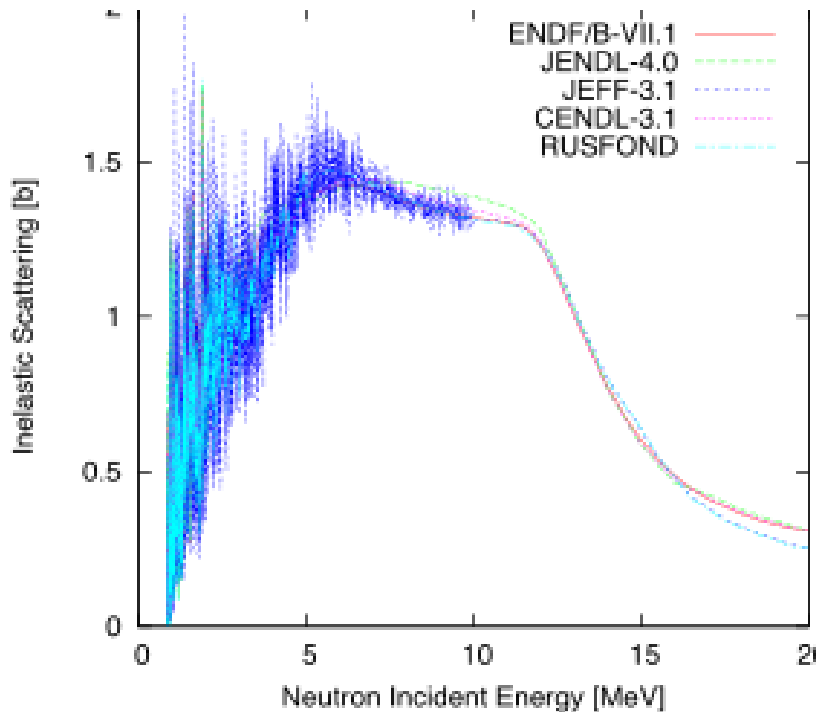
- Geel data below 6 MeV accurate and consistent with new evals

Performance in iron benchmarks ~ acceptable/good (“no worse!”)

Independent evaluation studies from China tend to corroborate conclusions



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



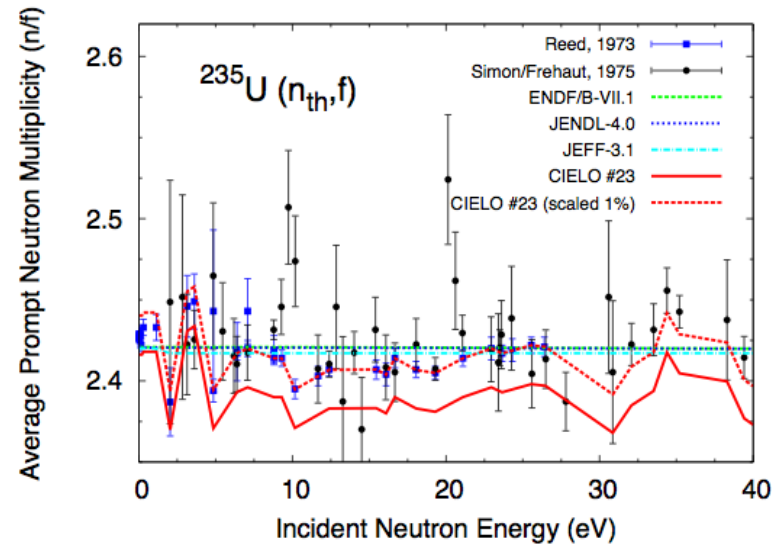
Herman, Palmiotti

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

# 235 nubar? iaea

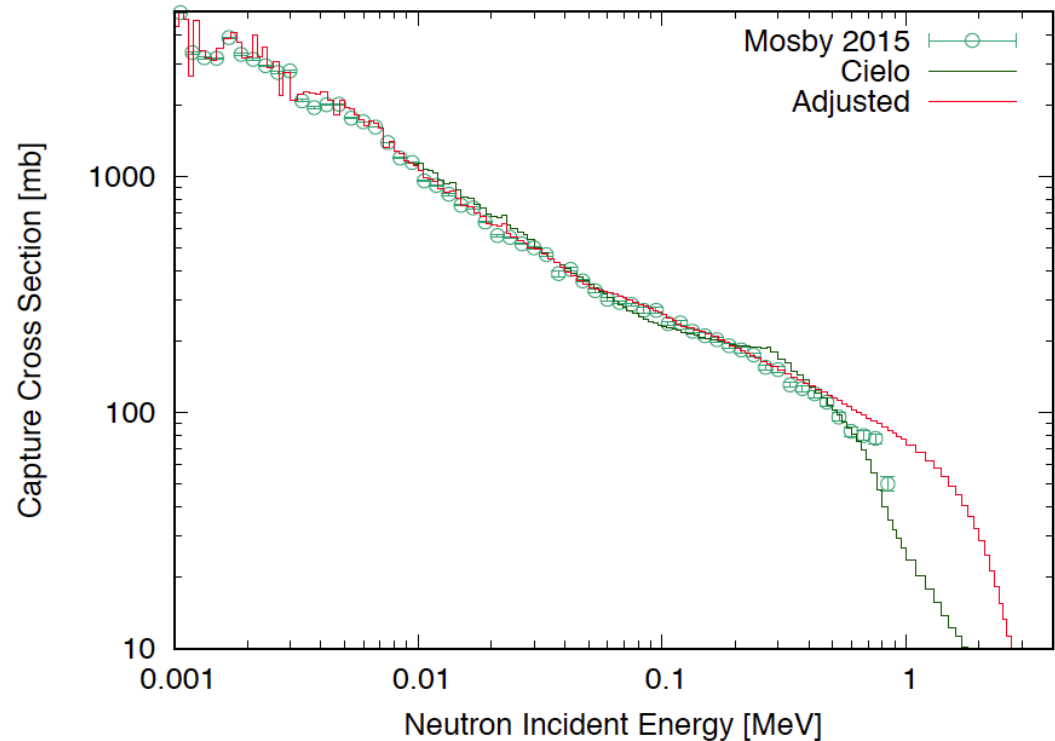
## Prompt Neutron Multiplicity

- From IAEA's latest file:
  - "Prompt nu-bar evaluated by V. Pronyaev, based on Reed data from C00-3058-39, normalized to thermal value of 2,41161. Simon data were measured rel. to  $^{252}\text{Cf}(sf)$  normalized at 10-27 eV on Reed's data (10-Jan-2016). The dip in the data around 30 eV was suppressed. Thermal value was increased by 0.0046 below 0.2 eV."



## DANCE Capture Data Test

- Mosby's data Oct. 2015
  - from URR to 1 MeV
  - URR parameters slightly adjusted
  - CoH3 calculation given to the high energy part
    - Soukhovitskii 2005 potential
    - fission adjusted
    - M1 scissors mode included
- CIELO file issue
  - Inelastic scattering exists in URR, but total does not have it
  - Cross section fixed from 9 to 30 keV



## Summary ...

CIELO collaboration is making progress in resolving open questions

Starter files created – being tested

Documentation to be completed in next year.



## Possible CIELO papers – NDS 2018?

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- ✦ Chadwick - short overview of CIELO SG40 objectives and accomplishments
- ✦ Hale et al -  $^{16}\text{O}$  evaluation ?
- ✦ Hale, Kunieda, Livermore collaborators, ...
- ✦ Broader O16 collaboration conclusions on magnitude of  $n,\alpha$  based on unitarity
- ✦ Georginis, Plompen et al - conclusions on  $^{16}\text{O}$  ( $n,\alpha$ ) corrections on historic data
- ✦ Plompen et al, the low energy  $^{16}\text{O}$  total elastic cross section
- ✦ Leal? - his R-matrix  $^{16}\text{O}$  evaluation (not in B-VIII)
- ✦ Herman et al - BNL staff - more details on  $^{56}\text{Fe}$  in fast region?
- ✦ Trkov et al - resonance region of  $^{56}\text{Fe}$
- ✦ Leal et al - new resonance analysis of  $^{56}\text{Fe}$
- ✦ Chinese work on  $^{56}\text{Fe}$  - eg inelastic scattering evaluation

## Possible CIELO papers –NDS 2018?

---

- ✦ Romain, Morillon, Bauge et al - CEA fast actinide evaluations
- ✦ Chinese work on  $^{235}\text{U}$
- ✦ M.Pigni et al (Trkov) resonance analysis of  $^{235}\text{U}$
- ✦ R. Capote et al, fast  $^{235}\text{U}$  and  $^{238}\text{U}$  analysis
- ✦ L. Leal resonance analysis of  $^{235}\text{U}$
- ✦ Schillebeeckx et al., new Geel  $^{238}\text{U}$  resonance analysis - MBC notes not yet in B-VIII-beta1
- ✦ Kawano -  $^{238}\text{U}$  and LANSCE capture theory and model calculations
- ✦ Neudecker - PFNS evaluations of actinides - incl those that did not make it into B-VIII, eg thermal  $^{239}\text{Pu}$
- ✦ Talou - multiplicity dependent fission neutrons and gamma-rays
- ✦ Kawano, Capote, Romain, et al, latest conclusions on actinide inelastic cross sections

# CIELO NDS 2018 Template

## Neutron reaction on XXX under the CIELO Collaboration

author<sup>1,\*</sup>

<sup>1</sup>Lab address

(Dated: April 29, 2016)

Abstract.

Note we do not yet know page restrictions for these individual CIELO papers, but plan for somewhere between 4-10 pages each. (The same ND2018 issue will have a large 100+ paper on ENDF/B-VIII, and a large 30+ page paper on new standards). Thus we expect perhaps 150 pages reserved for separate CIELO papers.

### I. INTRODUCTION

The paper should be journal quality; it will be peer reviewed.

Give background, e.g. - The CIELO pilot project was commissioned by the OECD's Nuclear Energy Agency WPEC (Working Party on International Nuclear Data Evaluation Co-operation) during a meeting held in May 2012. The goal has been to identify deficiencies and discrepancies in our current understanding of neutron reactions on high priority nuclides  $^1\text{H}$ ,  $^{16}\text{O}$ ,  $^{56}\text{Fe}$ ,  $^{235}\text{U}$ ,  $^{238}\text{U}$  and  $^{239}\text{Pu}$ , and to develop proposed solutions and improvements in our understanding. The goals of CIELO are documented in Ref. [? ]. This reference, together with other papers such as Refs. [? ? ? ] document some of the questions being addressed.

Explain clearly which isotope and cross sections or energy/angle distributions will be addressed.

Explain the background as to why our previous understanding was inadequate. Why - a lack of accurate experimental data? Insufficiently reli-

able model predictions? What were the assessed uncertainties prior to the present work?

Possibly summarize the applications that have motivated the work.

### II. RESULTS

Explain the basis for your new conclusions - new experiments made, theory, new analyses?

What are your new proposed uncertainties?

Proposed or recommended evaluations should (a) provide a ENDF-formatted file that can be archived on the NEA CIELO web site; and (b) be documented in this paper, with illustrative figures that compare the recommendation against the main evaluated data libraries, such as ENDF/B-VII.1 [? ? ], JEFF-3.1 [? ? ], JENDL-4.0 [? ], BROND/ROSFOND [? ], and CENDL-3.1 [? ].

What are remaining open questions that remain unsolved?.

# BACKUP SLIDES

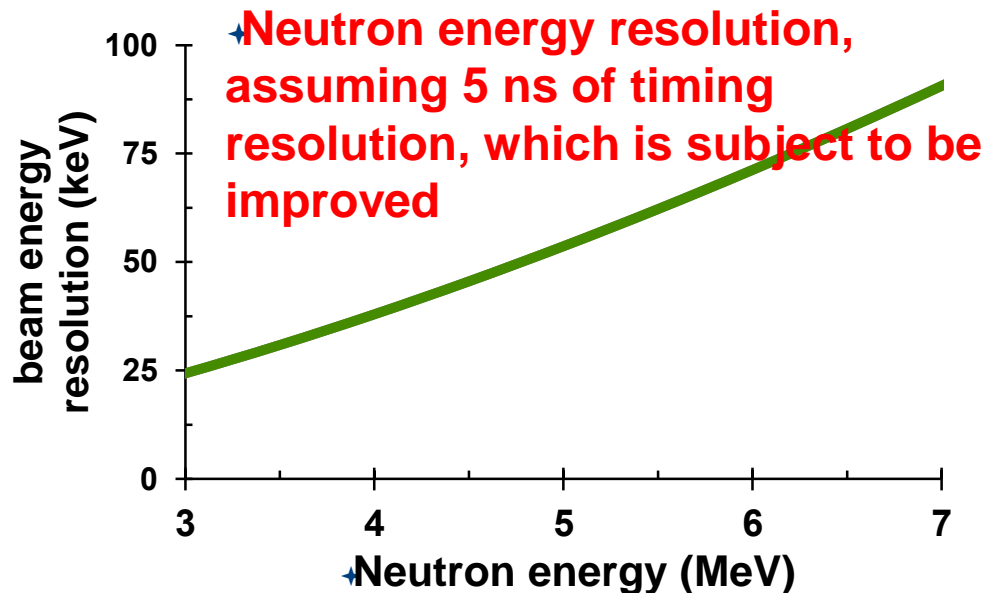
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Cecil Lubitz:

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

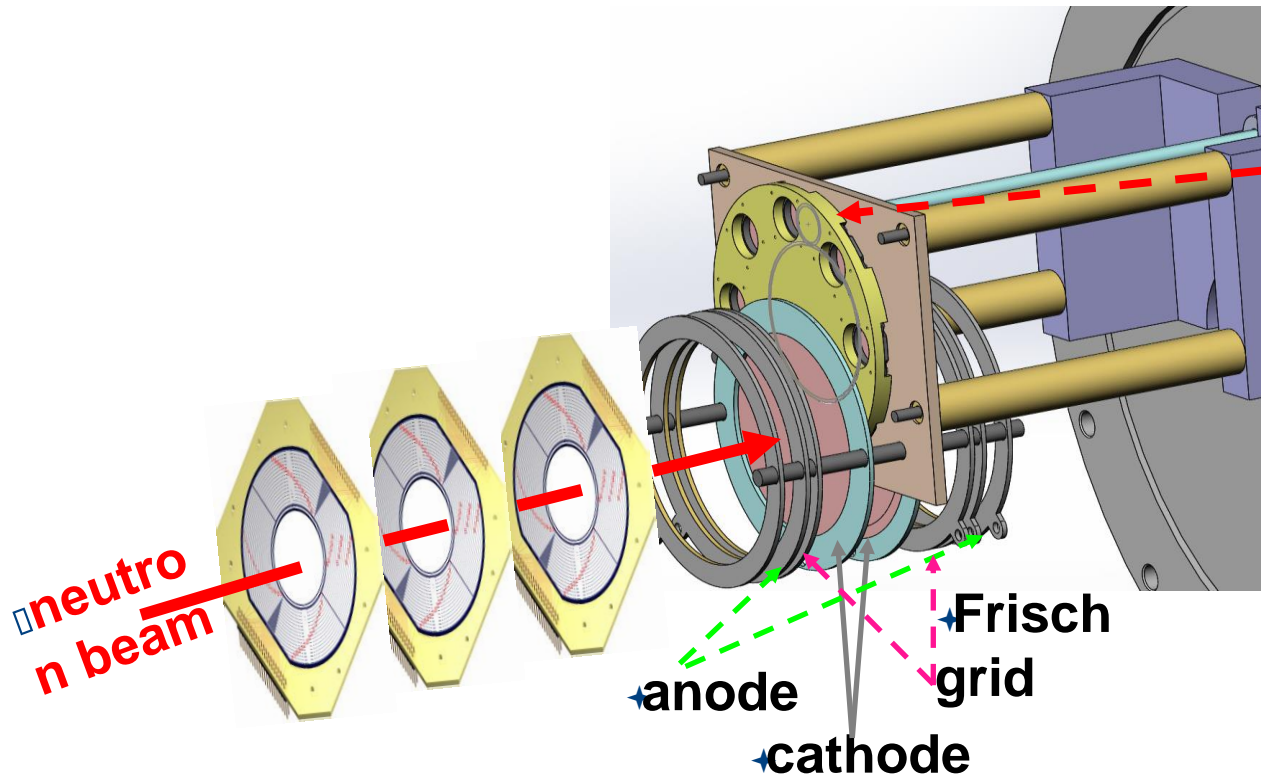
# LANL plans to measure new cross sections on $^{16}\text{O}(n, \gamma)$

- 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.

160

General

Intercompare evaluations, and identify goals for a new evaluation

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  
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

Total, Elastic and Inelastic scattering

Compare existing evaluations and R-matrix analysis, and define path forward

At low energies, assess whether evaluations of elastic scattering indeed need to be lowered by ~3%, as proposed by Plompen, Lubitz, Roubtsov etc

covariances for mubar: Need reliable anisotropic 16O scattering uncertainties. Palmiotti thinks Gerry's present uncertainties are too small on mubar.

Capture

ENDF adopted JENDL's capture cross section to include resonance contribution - establish consensus to use this

(n,a)

Review different evaluations (all largely same as ENDF)

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?

Review new data - Georginis (Geel), Khryachkov (IPPE) - contact physicists working on 13C(a,n) for astrophysics

The above new data approx confirm ENDF below 6 MeV but point to changes above

Intercompare R-matrix calcs (Hale, Kunieda, Leal)

Seek to understand why the above R-matrix evaluations, influenced by total cross sec data, suggest ~30% higher (n,a) than most measurements

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

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

Integral

Establish suite of integral validation tests, including k-eff, transmission, etc

2 benchmarks sensitive to oxygen data (+11 more benchmarks with water) are available in the SINBAD database

Broomstick experiment

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

(n,a) impact at higher energies: Does this higher energy >6 MeV region impact any applications significantly (maybe medical applications)? Carlson notes M

check astrophysics constraints on 13C(a,n) reaction rate

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

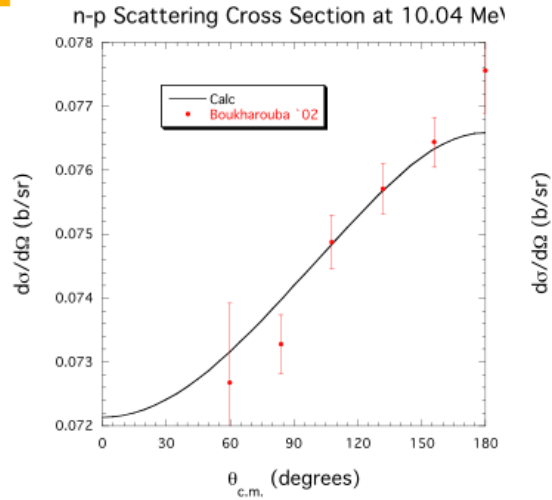
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- **NN analysis progressing; more p-p elastic scattering data needed in the 30-50 MeV range. Low-energy parameters retain their earlier (correct) values. Need to extend analysis above 200 MeV.**
- **New data for n+<sup>6</sup>Li fit in well with the 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.**

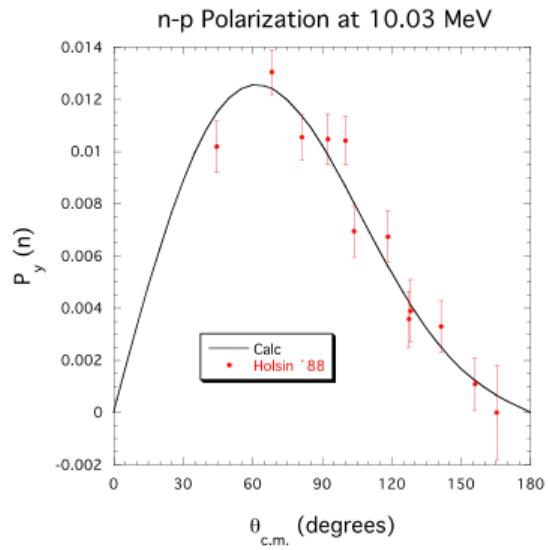
# **$^1\text{H}$ – Hale comments on the covariance data**

*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



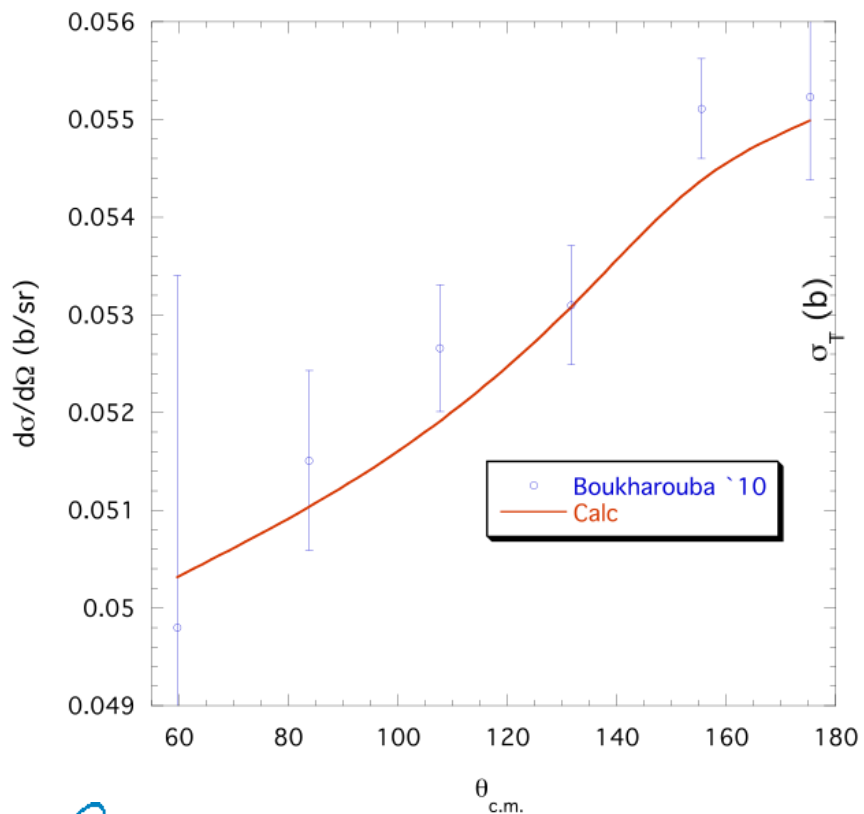
# n-p Polarizations



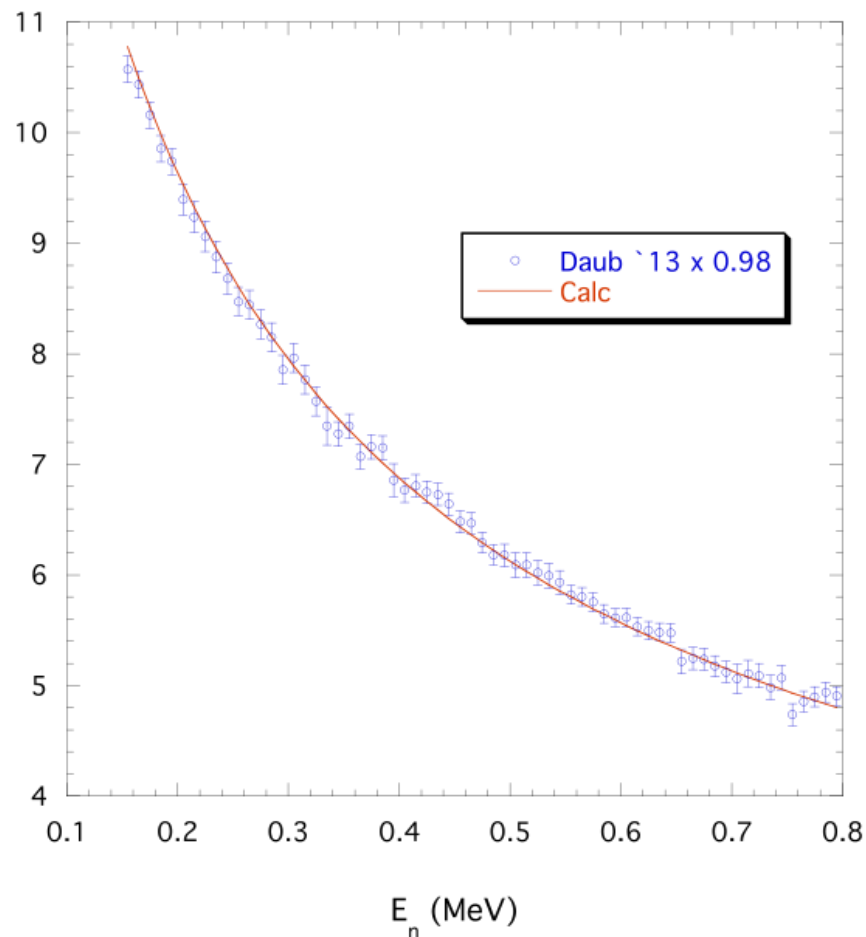
$P_y(n)$

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

n-p Differential Cross Section at 14.9 MeV



n-p Total Cross Section



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	<b>Fast Region (keVs and above to 20 MeV) - fission listed separately</b>		
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 – II. Prelim LANL testing of new Subgroup 34 resonance results

- **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  $k_{\text{calc}}$  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  $k_{\text{calc}}$  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>

a) MCNP calculations are for 250M histories; stochastic uncertainty is ~5 pcm.  
b) JEFF-3.1.2 and JENDL-4.0  $^{239}\text{Pu}$  only; remaining nuclides are ENDF/B-VII.1  
c) “LEAL7a” evaluation provides revised resolved resonance parameters coupled to a joint ORNL/CEA evaluated  $^{239}\text{Pu}$  file; the “LEAL7a (RR,nu,pfns)” file couples just these data to the existing ENDF/B-VII.1  $^{239}\text{Pu}$  file.

# 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 2014-2016 Years:

- Various collaboration meetings, continual email collaborative exchanges
- engagement with validation data testers continually
- Start incorporating 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, 2018)
- Create formatted files that embody CIELO's initial conclusions