



## **Evaluation of pre-ENDF/B-VIII Cross Section**

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**Thx to many many for input.**

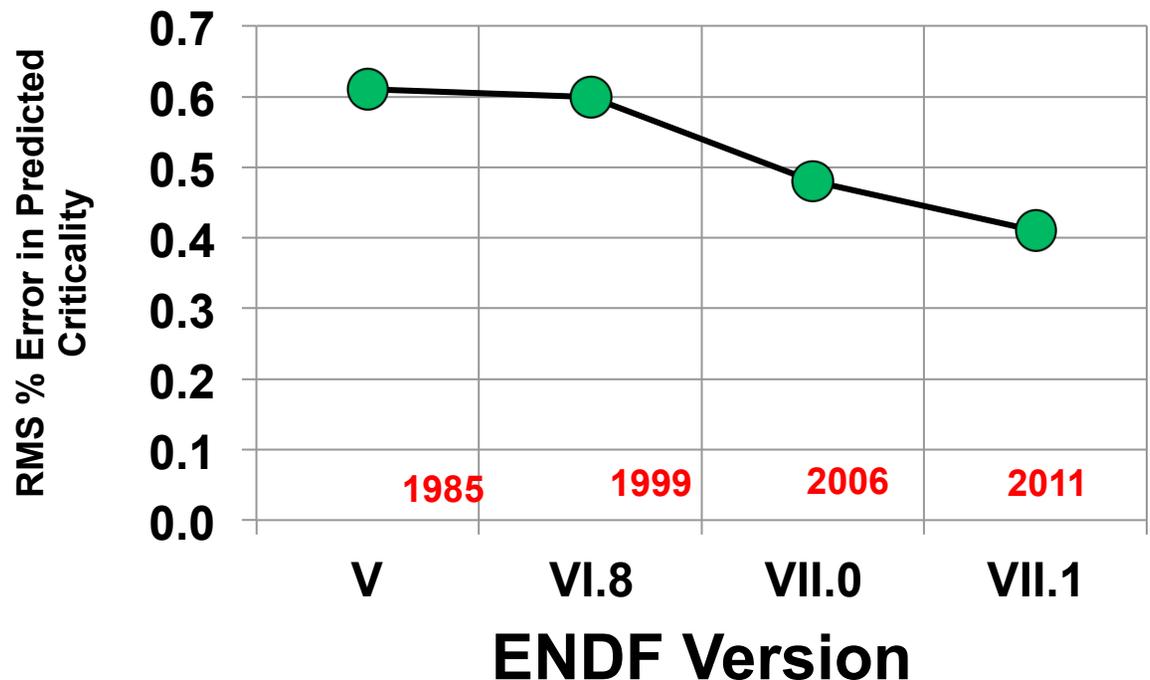
CSEWG Meeting, Brookhaven, November 2, 2015



# ENDF/B-VII.8 Goal is to advance our database for the most impactful isotopes – actinides, iron, oxygen, ... – using CIELO work

- » **Numerous fundamental cross section advances**
  - » Resonances
  - » Fast region capture, fission, scattering, .... nubar, PFNS spectra ...
  - » Standards
- » **Challenge is to preserve and improve integral **criticality, transport, & spectral index** performance**
- » **For example our new:**
  - » U235 IAEA thermal PFNS incr. thermal criticality
  - » <sup>16</sup>O Hale n, alpha lowers thermal criticality

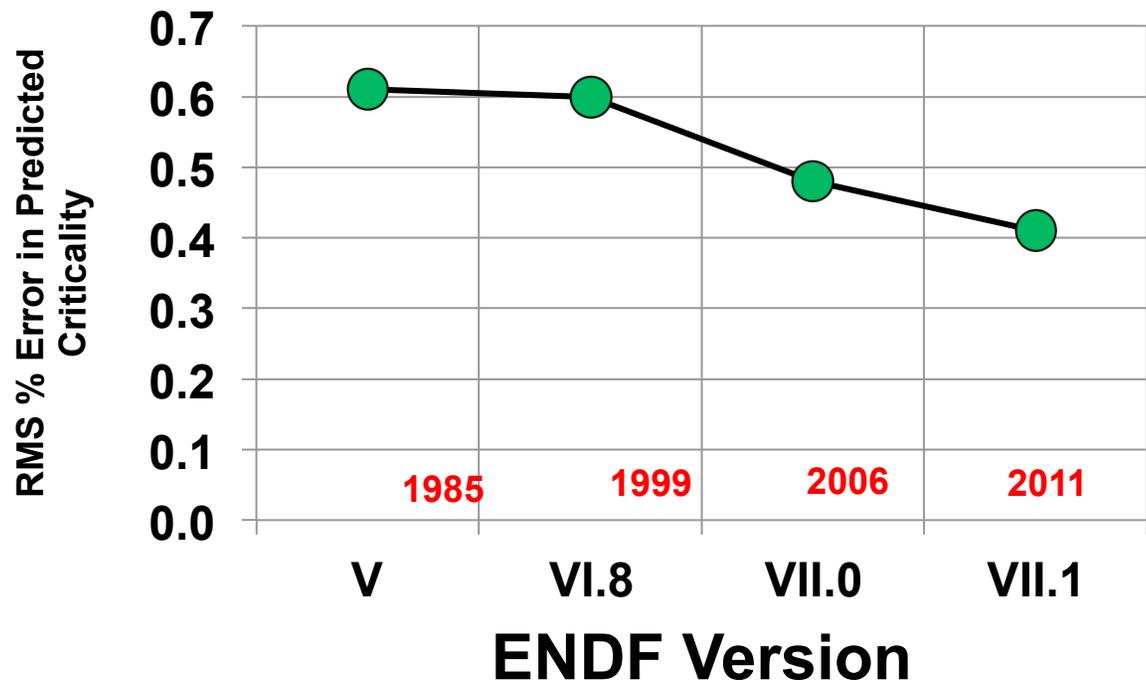
“Mosteller” suite of 119 critical assemblies that we track over time (MCNP6 calculations)



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Pre-VIII.CSEWG.Nov2015 for 235,8U,239Pu,16O changes from 0.42% to 0.44% (Forrest Brown) - Not too bad!

Jedrowski

# Plan for Reaching ENDF/B-VIII Release in 2018

## Higher risk:

- Inelastic scattering
- Capture in fast region
- More PFNS upgrades
- ...

END/B-VIII.0 2017/18  
- Further major upgrades

## Pre-ENDF/B-VIII, 2015

- Base upgrades established (covariances not yet added)
- + numerous variants
- **1H, 16O, 56Fe, 235,8U, 239Pu,**
- 9Be?, C, Ne, Ca, Ni, Cu, As, Re, W, ...
- Thermal kernels (SG42)

CIELO help

END/B-VIII.0 2017/18  
- Modest upgrades

## Low risk:

- Fission product yields, TKE
- PFGS (fission gammas)
- PFNU (nu)
- ...

END/B-VII.1, 2011  
- Widely used in DOE & around world

# Summary of Data Testing of new pre-VIII.CSEWG.Nov15 Files (u5=19c ; u8=4c=iaea ib44 ; o16=5c=halead; pu9=23c) cf. VII.1

## » **Fast region:**

- » Unreflected: Jezebel, Godiva (~equally good)
- » Pu & HEU Flattops (a bit worse. 238U reflection?)
- » Bigten (a bit worse)

## » **Thermal region:**

- » Pu solutions – much better
- » U5 solutions – reasonably good. Plotted against above-thermal-leakage shows a good intercept (small positive bias slope reduced with new o16..)
- » LEU worse (LCT5,7 down av. 150 pcm, per Kahler) - u8, o16 impact?

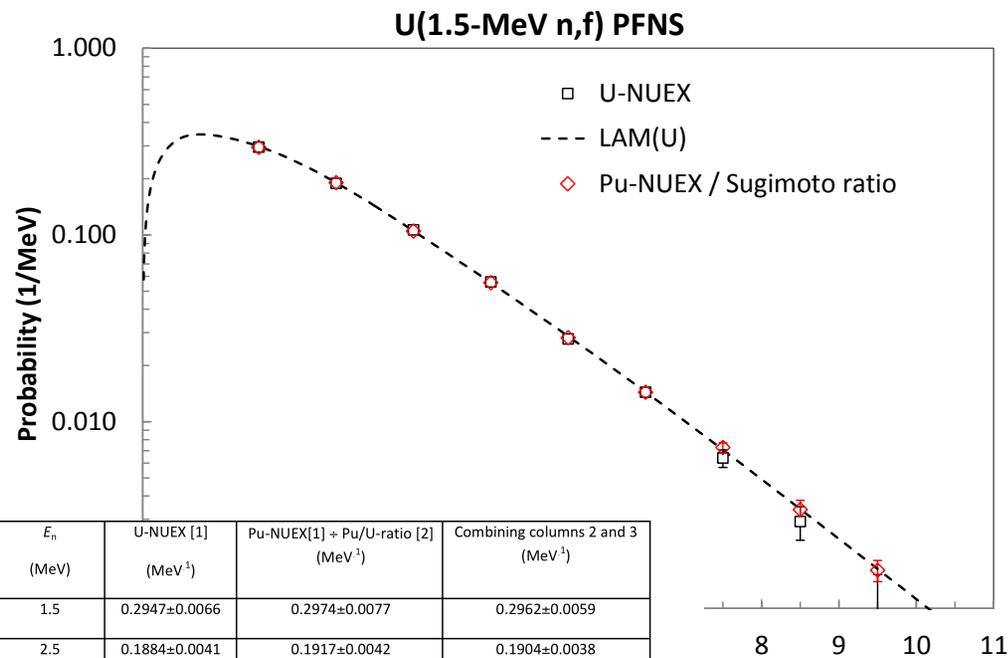
**Phase space of evaluation trial files, for testing, is very large. Much ENDF testing work done by Kahler (LANL) and Trkov, Capote (IAEA):**

- **Single Substitutions of new files into VII.1**
- **Substitutions of ensembles into VII.1 (u5,8,pu9,o16, ...)**

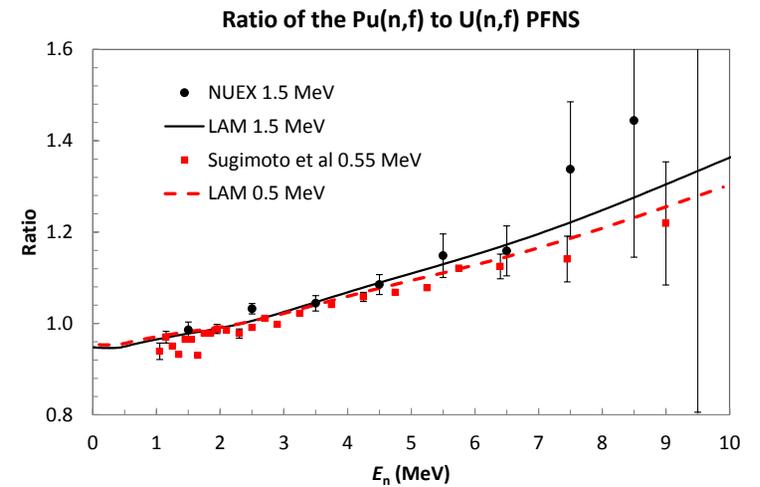
## 235U pre-VIII file, NAME=19c

- » Updates near 2 keV using Leal et al resonances, based on LANSCE /DANCE & RPI data, & lower-energy resonance changes to fit thermal  $\sigma_f, \sigma_\gamma$  STD micro fit & nubar changes: *i.e.* Low energy part of IAEA file u235ib02i2g6cnu3f2
- » Prompt Fission Neutron Spectra
  - » Adopt IAEA thermal spectrum evaluation,  $E_{av}=2.00$  MeV (versus 2.03 MeV)
  - » Above thermal, Rising-Talou evaluation to 5 MeV (matches Chi-nu & NUEX)
- » **Known Issues not yet addressed:**
  - » A major IAEA upgrade, including fast energies may reach maturity ...
  - » Nubar near thermal and above needs attention (mean values, fluct)
  - » Res. integral in 7.8-11 eV incr 2% ~246 beV (Carlson; Leal). V&V-ing in progress
  - » Capture updates may be needed in 10s of keV region (and above?) based on DANCE, Wallner data. New data coming with NEUANCE.
  - » Kawano, Capote et al are studying inelastic models & evaluation updates, with future use of RPI-type semi-integral scattering data
  - » PFGs; P(nu), Chi(nu); TKE updates; FPY TUNL updates esp at 14 MeV.
  - » Data testing of void reactivity (Japanese help?); Criticality performance?

# $^{235}\text{U}$ : NUEX continued studies for $^{235}\text{U}$ , Lestone, Shores, Impacting our $^{235}\text{U}$ PFNS evaluation

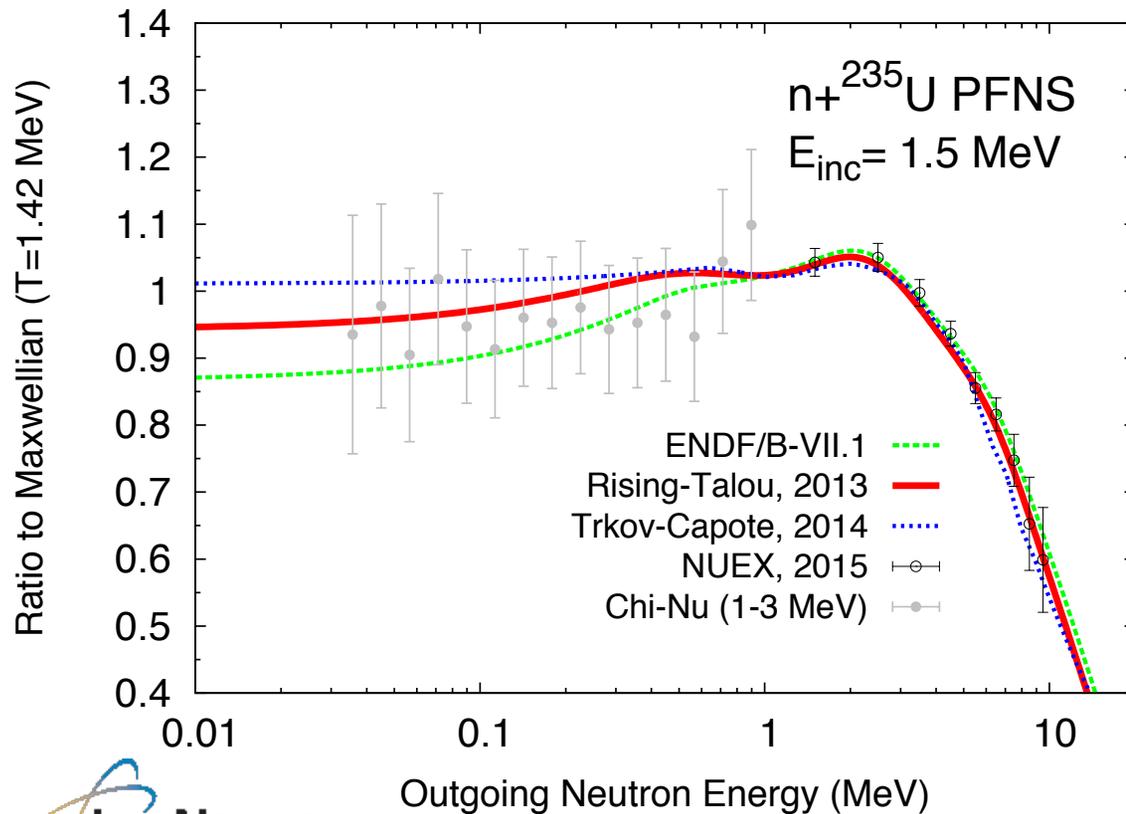


**Fairly good agreement between Los Alamos NUEX PU/U ratio, compared to lab ANL measurements**

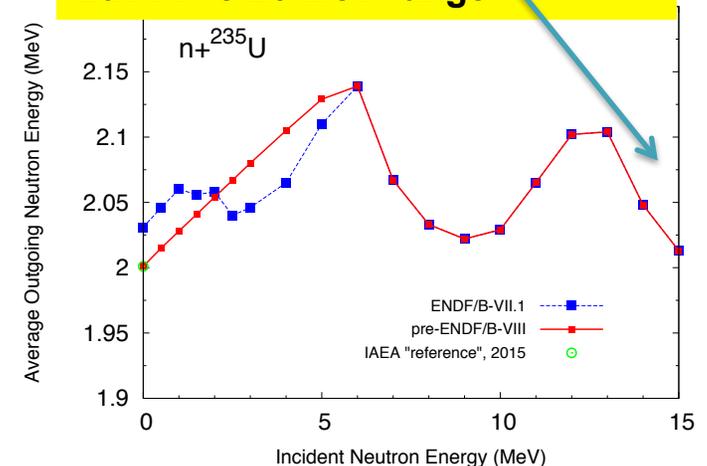


# $^{235}\text{U}$ : Two LANL experiments cover the whole emission energy range – Chi-nu (LANSCE) and NUEX (Lestone-Shores)

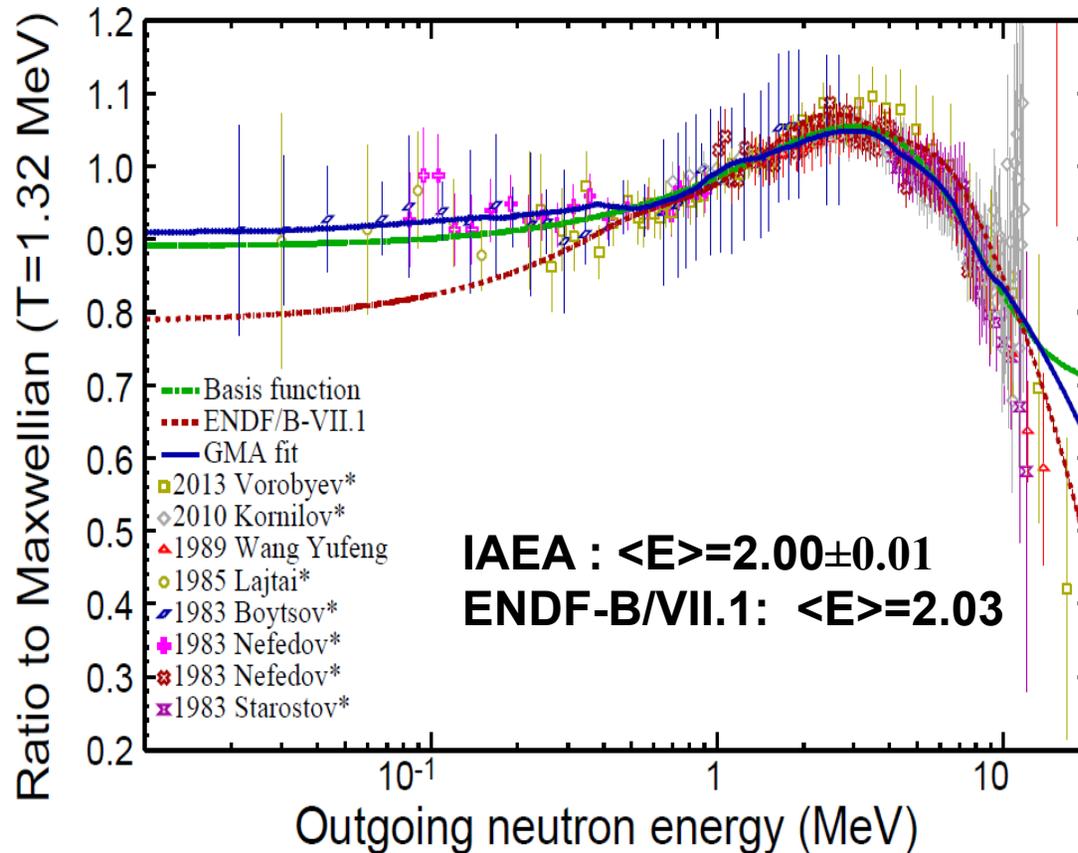
Talou-Rising is a bit different to the IAEA PFNS  
0.5-2 MeV – but not a lot



Previous VII.1 unphysical (?)  
structure in few-MeV range  
removed.  
A future upgrade will increase  
 $E_{\text{av}}$  in 15-20 MeV range

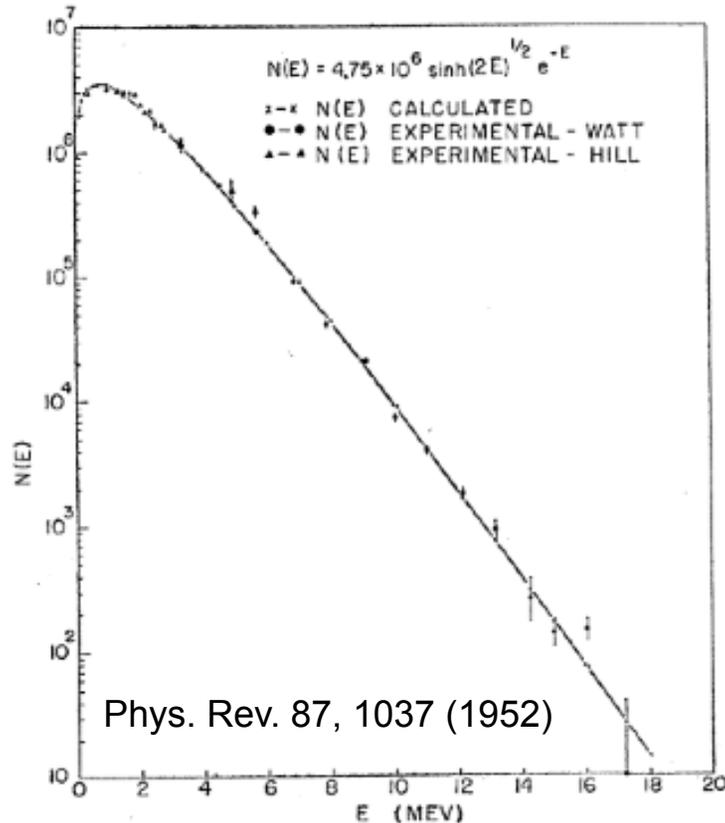


# $^{235}\text{U}$ thermal PFNS adopted from IAEA Standards work. Changing from $E_{av}$ 2.03 to 2.00 MeV has major implications



**We are adopting this work owing to the significant quality effort devoted; it increases thermal criticality. Other changes to  $^{235}\text{U}$  resonances, nubar, and 160 compensate for the change**

# $^{235}\text{U}$ thermal PFNS adopted from IAEA Standards work. New $E_{av}=2.00$ MeV agrees with Watt's LANL 1952 Analysis!



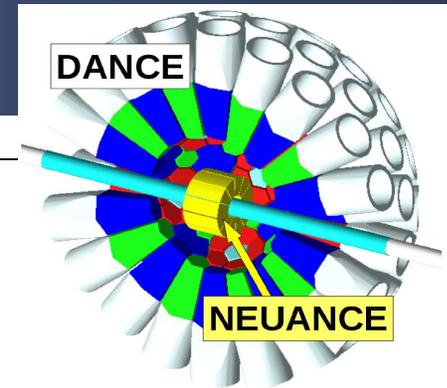
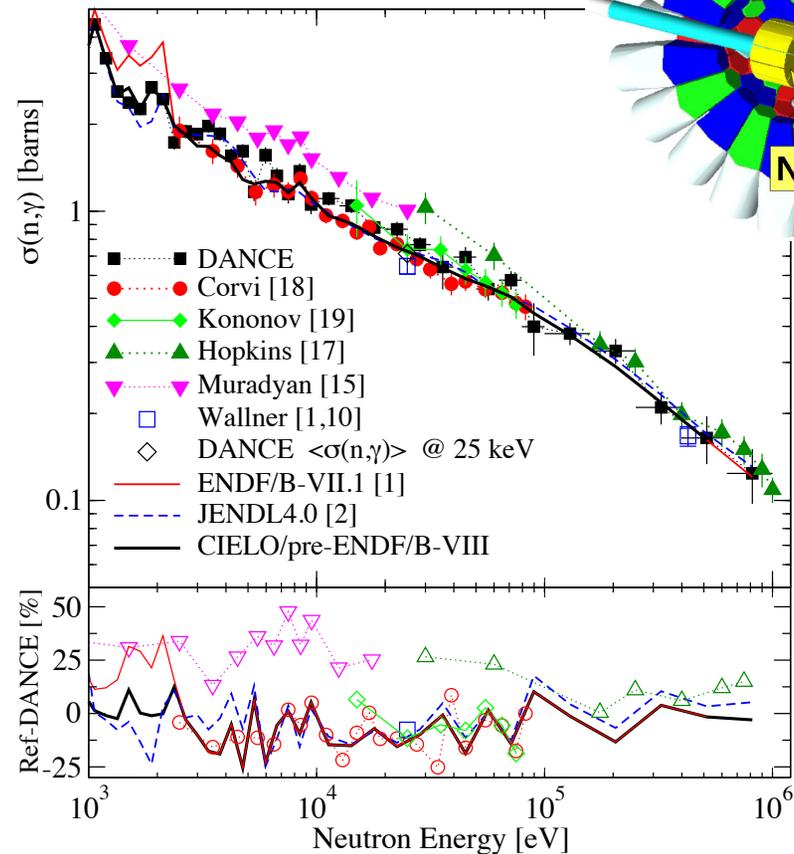
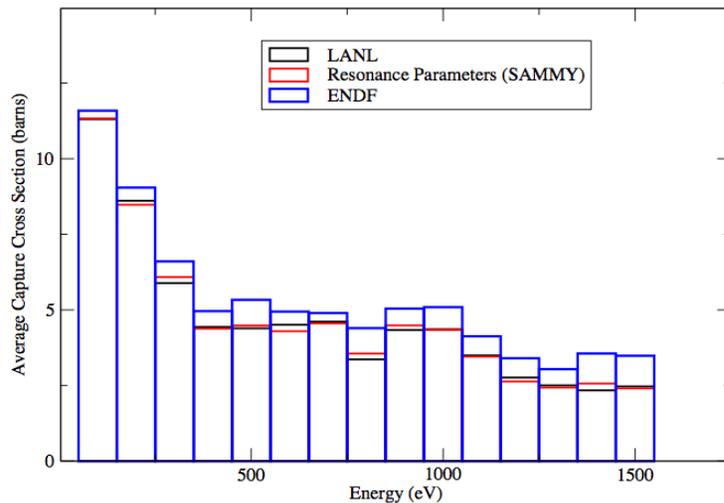
Watt spectrum:  $N(E) \sim \exp(-E/a) \cdot \sinh(\sqrt{b \cdot E})$   
 $E_{av} = (3/2)(1 + a \cdot b / 6)$ . (Broadhead, ORNL, PHYSOR2004)  
 $a=1, b=2$   
 $E_{av}=2.00$  MeV

FIG. 4. Energy spectrum of fission neutrons. The calculated curve is based on the assumption of a Maxwellian distribution in the center-of-mass system for the neutrons emitted by a fission fragment.

# 235U capture

» RPI and DANCE Capture data agree and have impacted new SAMMY analysis

U-235 SAMMY fitting of LANL Capture Data

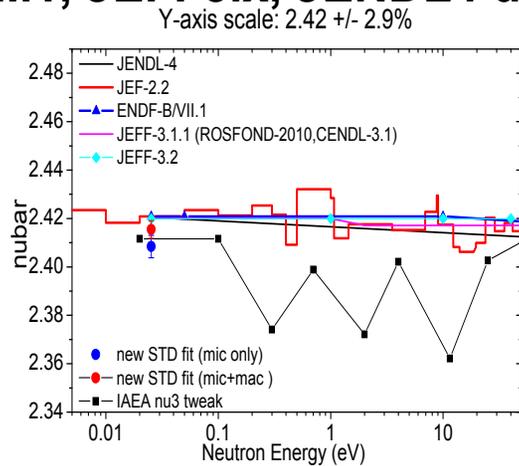


No change yet above a few keV, since ENDF represents the data reasonably well and recent AMS (Wallner) and DANCE data different. Forthcoming NUANCE data at LANSCE should further increase the data accuracy

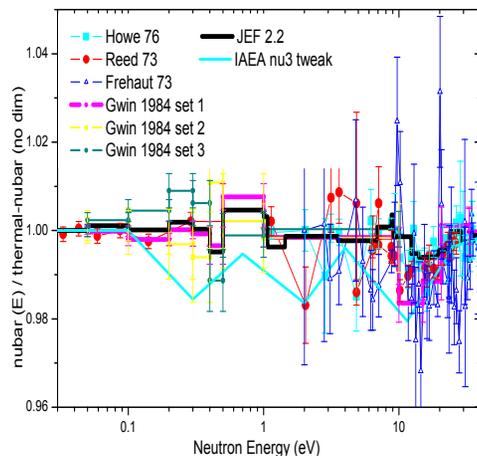
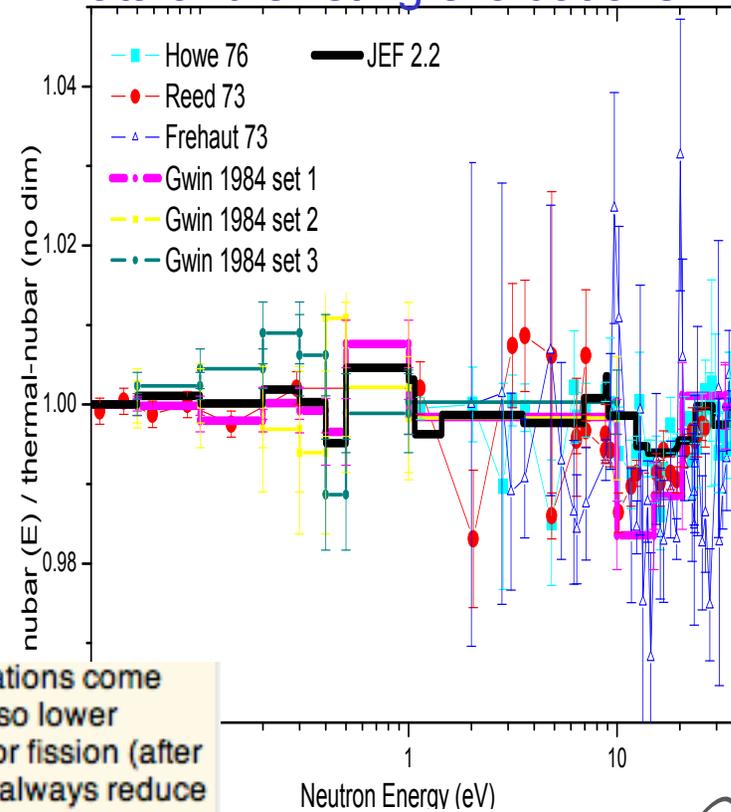
# 235U nubar - IAEA studying fluctuations

Both nubar fluctuations and resonance alpha (capture/fission ratio) below 20 eV have strong impact on the Keff vs ATLF trend. Luiz may find a solution where resonance alpha is larger for low-energy resonances, and we may reduce nubar fluctuations.

- » Uses this trial “nu3” nubar file from IAEA – but more work needed
- » VII.1, JEFF3.x, JENDL4 do not use fluctuations



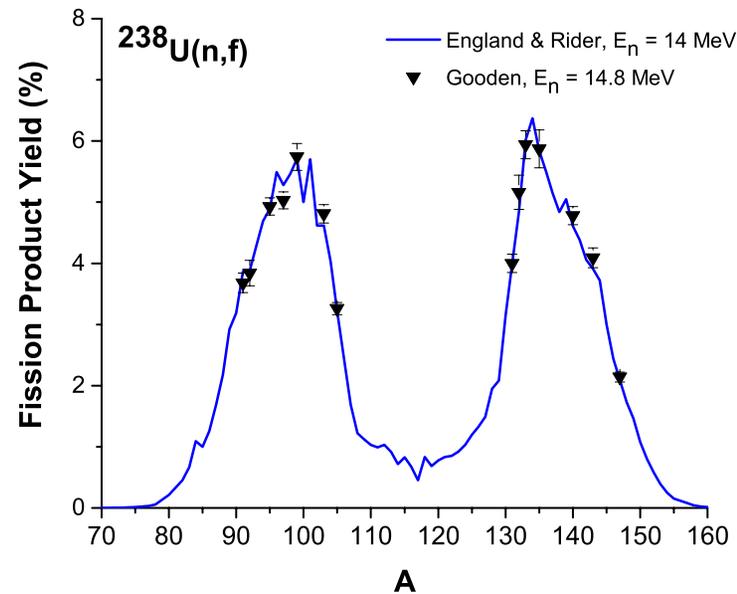
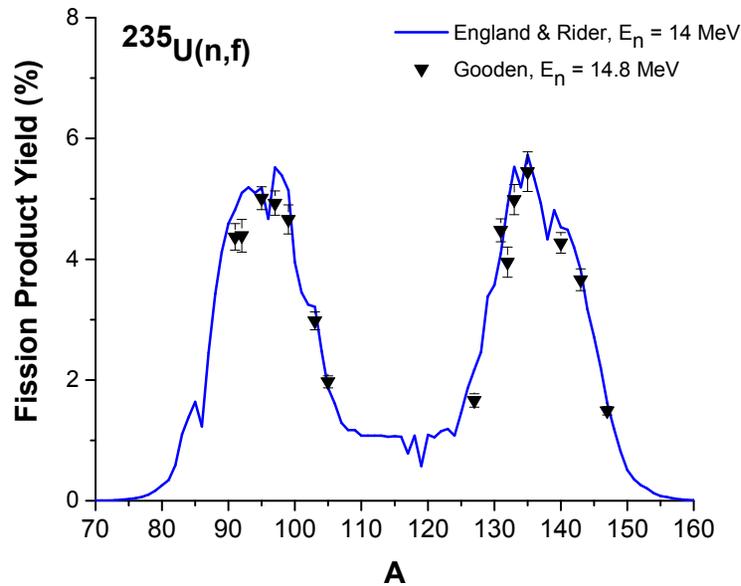
## Data and existing evaluations



Note: nubar fluctuations come from n,gf process, so lower energy available for fission (after gamma emission) always reduce nubar.

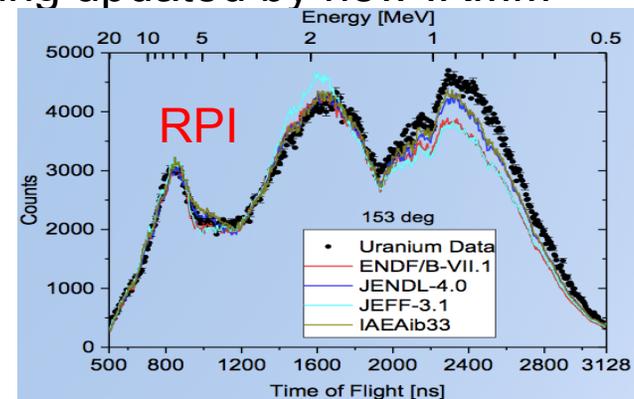
# 235U fission products

- » Update 14 MeV (and 0.5 MeV if needed) FPYs in ENDF, based on recent TUNL-LLNL-LANL Gooden *et al.* measurements



## 238U pre-VIII file, NAME=04c (IAEA ib44)

- » Major new 238U evaluation from IAEA, see talks by Capote & Trkov:
- » Includes:
  - » Inelastics from calculations and data (including RPI semi-integral data)
  - » Fission and Capture consistent with standards
  - » n,2n influenced by TUNL data
  - » Resonances adopted from B-VII, but being updated by new IRMM resonance analysis



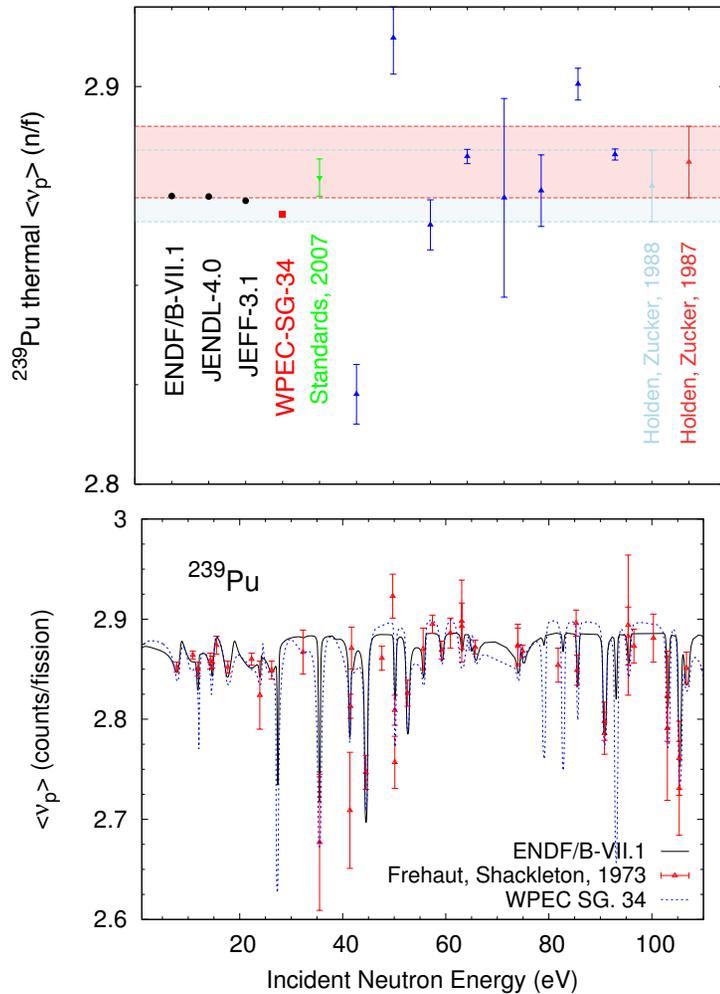
- » **Known Issues not yet addressed:**
  - » PFNS not yet changed. Some surprising results obtained at RPI and France regarding the spectrum shape below a few MeV – need confirmation
  - » TKE updates; FPY TUNL updates esp at 14 MeV.

## 239Pu pre-VIII file, NAME= "23c"

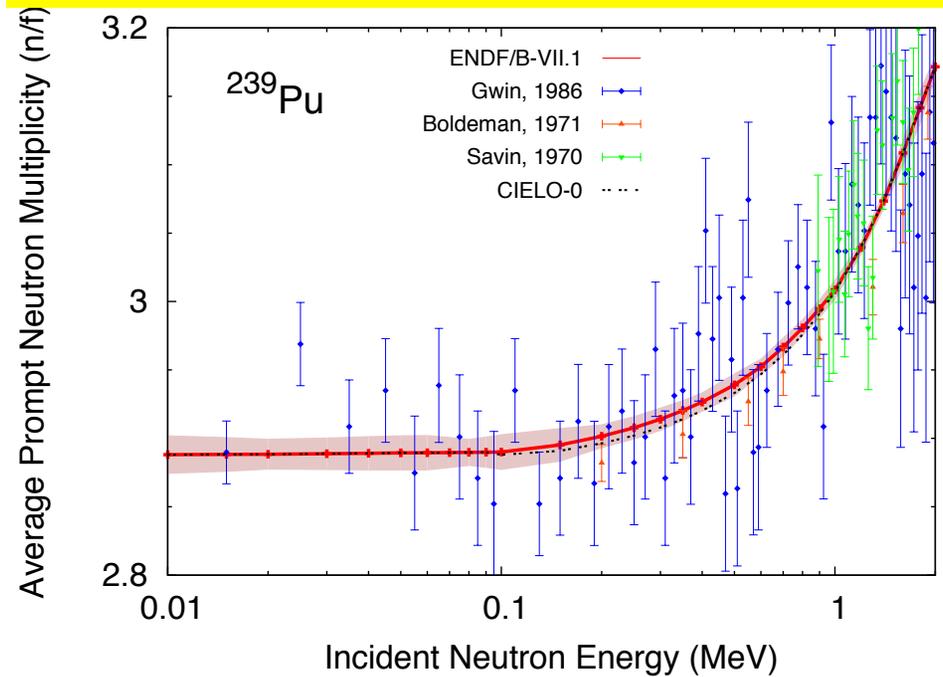
- » **NEA/WPEC SG34 resonances**
- » **SG34/JEFF3.2 nubar at low energies up to 650 eV, total nubar recalculated**
- » **PFNS > 5 MeV from LANL/Neudecker evaluation, ENDF < 5 MeV still VII.1**
- » **PFNS "Romano tweak" at thermal to better model thermal solution criticality**
- » **Old Young fast nubar tweak removed by Talou, now follows data**
- » **Huge section of delayed gammas removed**
- » **Known issues not yet addressed:**
  - » Unresolved resonances – consider use of ISSF=1 pointwise
  - » Leal resonances /capture up to 4 keV; Additional Leal work in resonances?
  - » Inelastics from calculations and data (including future RPI semi-integral data)
  - » Capture changes motivated by DANCE/NEUANCE – waiting for data
  - » Testing of Neudecker 14 MeV PFNS against pulsed sphere exp.
  - » PFNS data from Chi-nu ; add in TKE up to 14 and above; TUNL FPYs.
  - » PFGS and gamma-production in file6?; TPC fission – waiting for final data

# 239Pu nubar - both <650 eV; and fast range

SG34 nubar used appears low ...

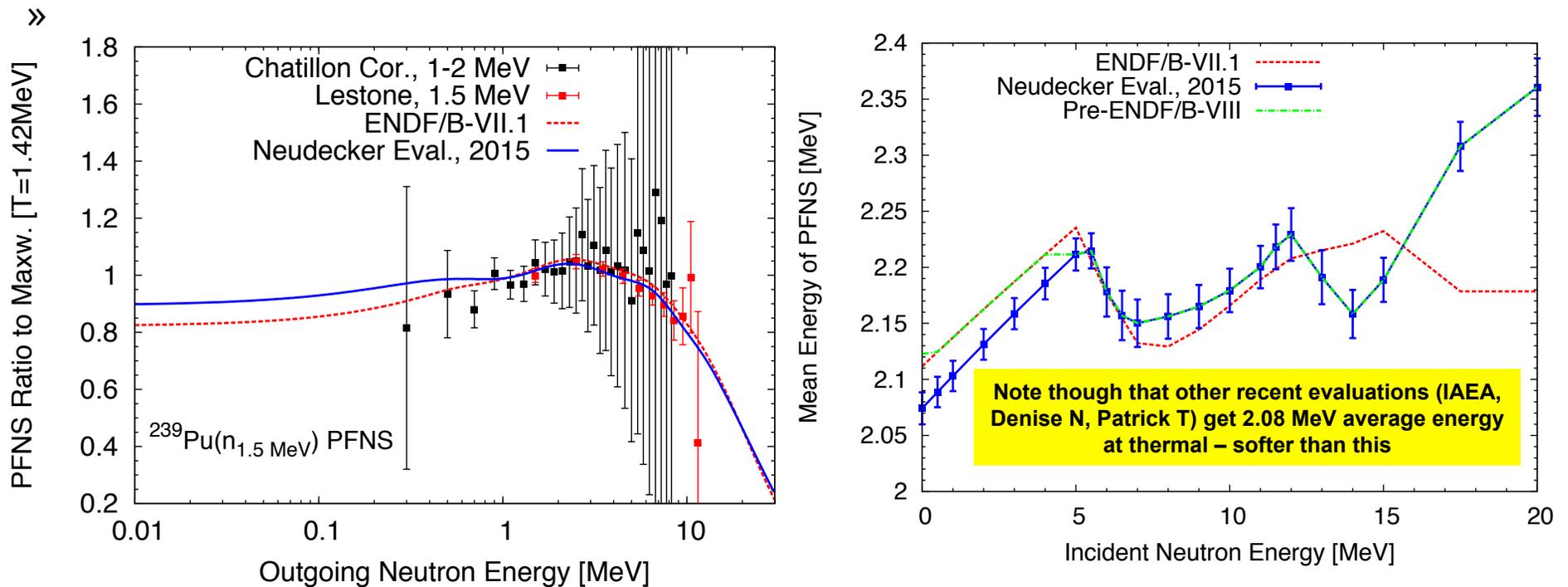


New fast nubar from Talou follows a covariance fit to data, and removes the higher tweak



# 239Pu PFNS: In fast region < 5 MeV, no change

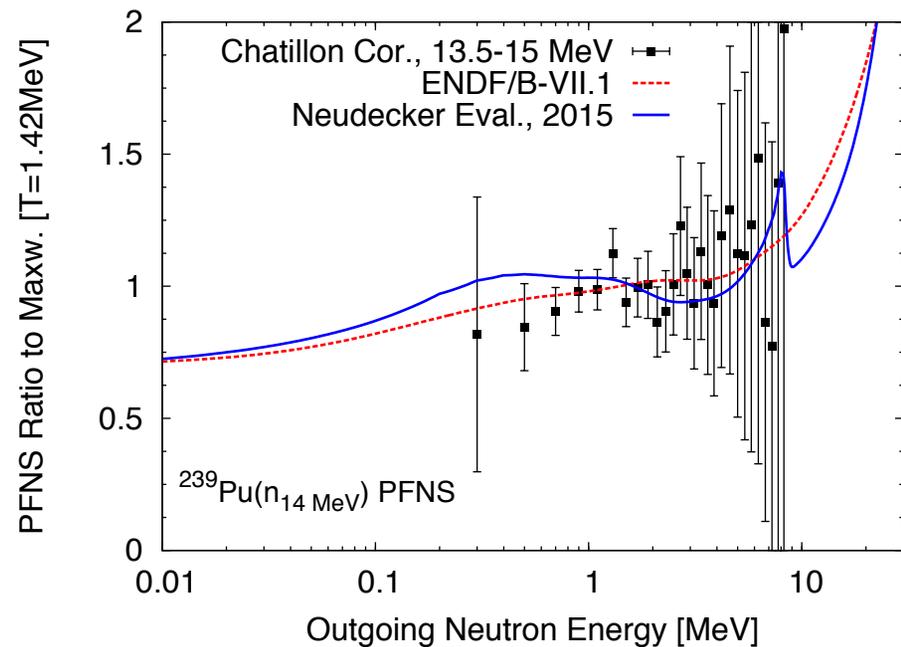
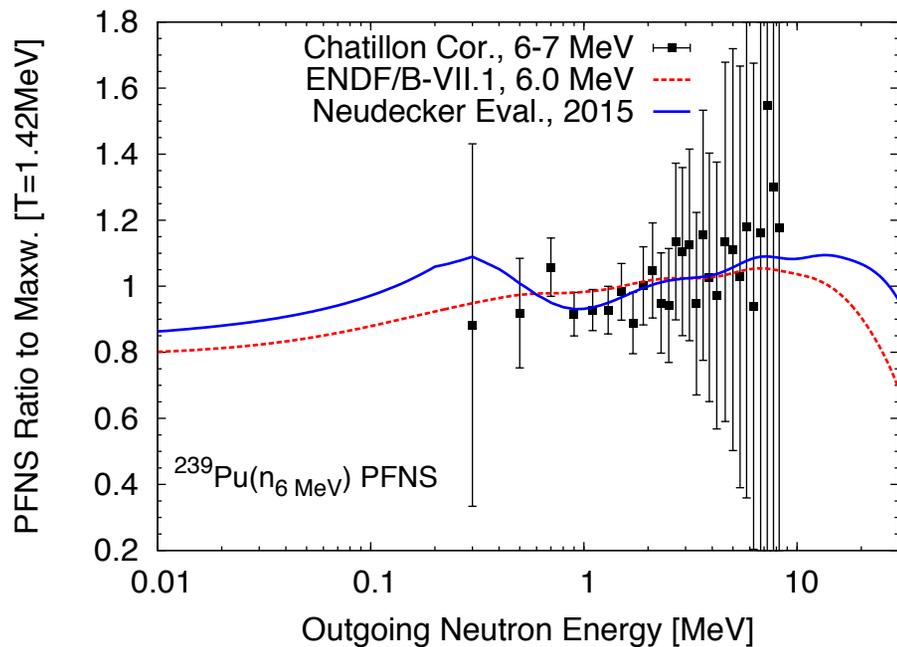
- » Above thermal and up to 5 MeV our pre-ENDF/B-VIII evaluation uses VII.1
- » Denise Neudecker's work is adopted only above 5 MeV.



It is premature to change the PFNS here, as we await Chi-nu data. The existing evaluation matches Lestone and Chatillon (Granier-mod.) data well, and performs well in integral simulations

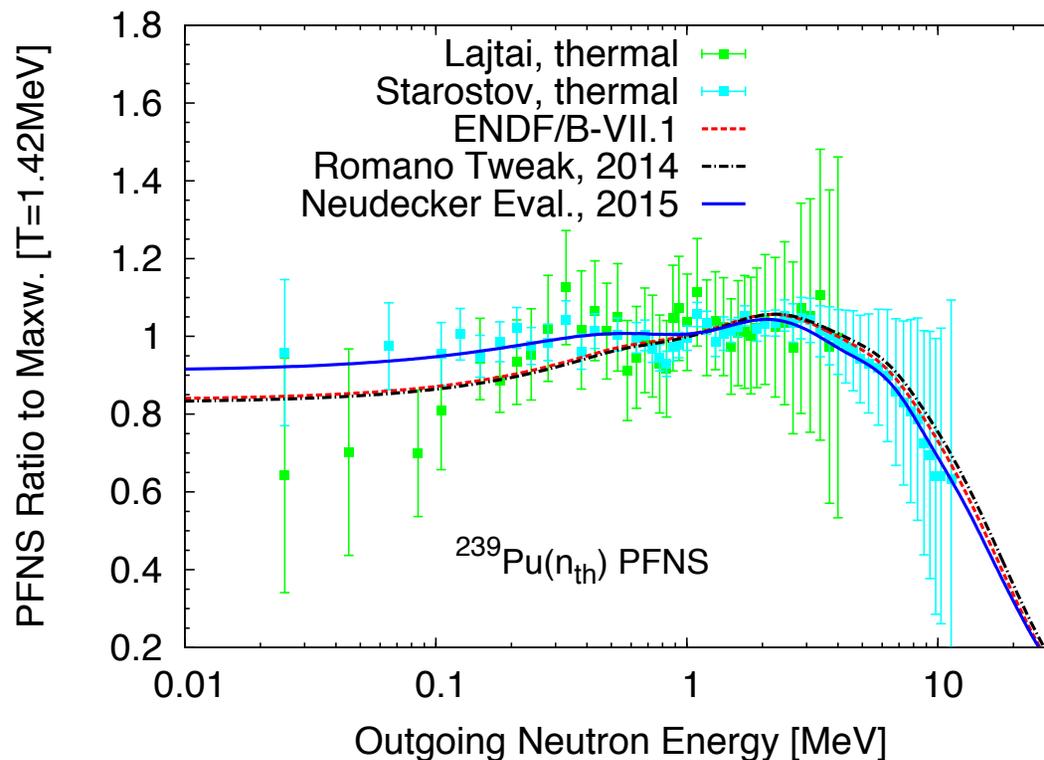
# 239Pu PFNS from 5-20 MeV from Neudecker Calculations and Evaluations

- » “Current” is adopted in pre-VIII. The new structure in these PFNS better characterize the multi-chance fission process, although it is not clear they better represent the Chatillon data!
- » We need to do integral data testing against 14 MeV Livermore pulsed spheres.



# 239Pu PFNS at Thermal

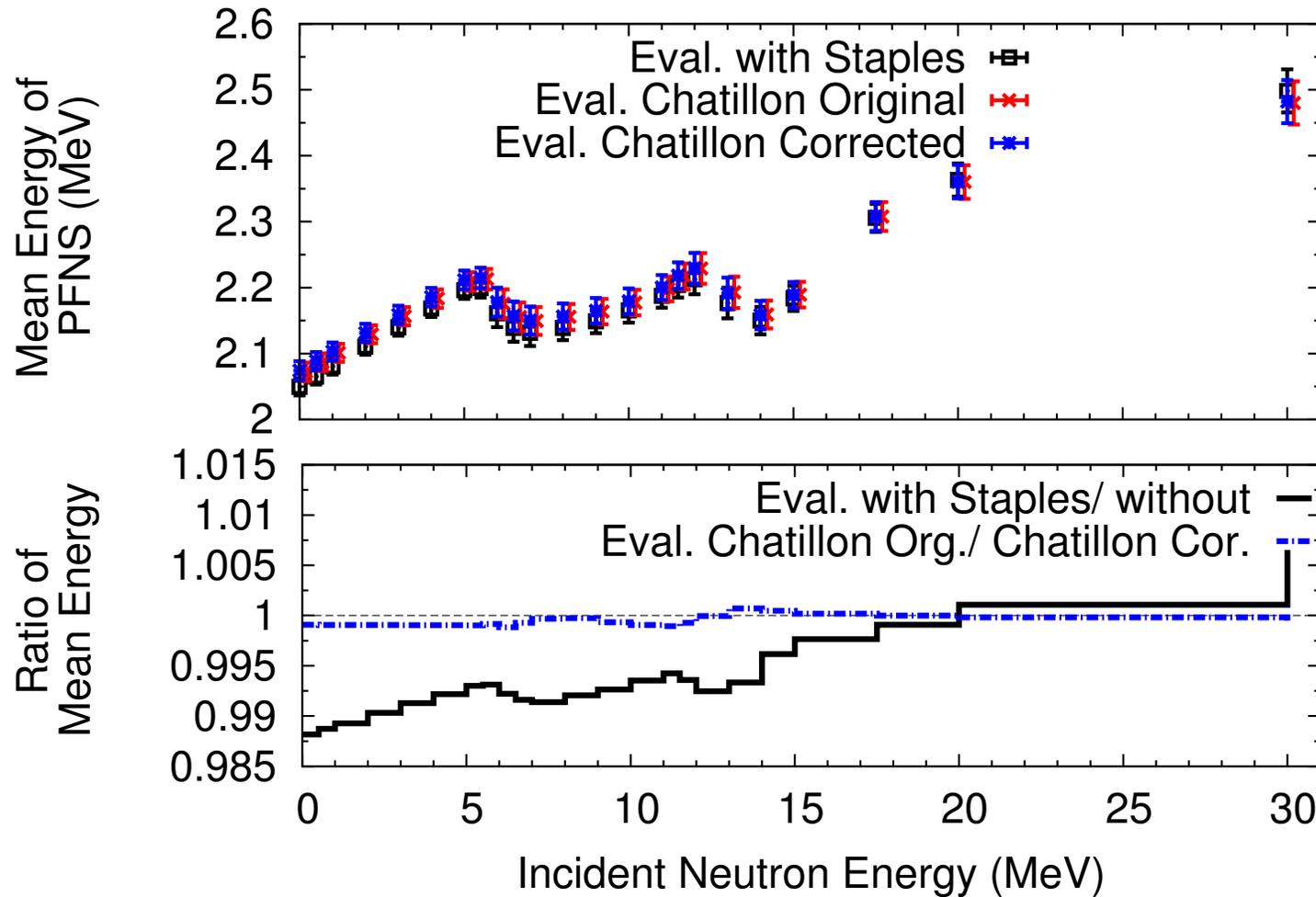
- » Romano tweak ~ invisible compared to VII.1
- » We await Chi-nu data before we want to change the evaluation here
- » Softening the PFNS will increase thermal criticality simulations, potentially removing the SG34 gains unless other changes are made



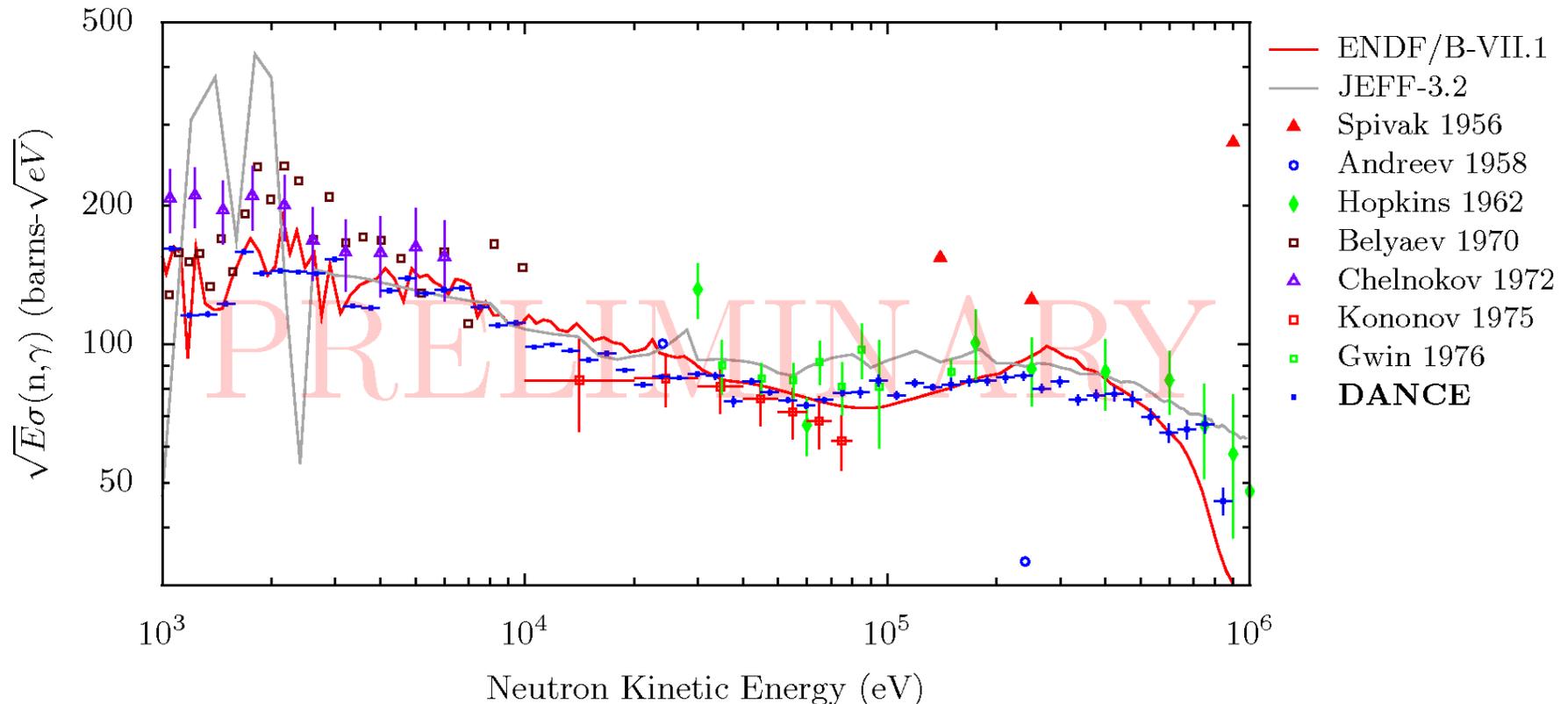
CAPOTE...rto Mario 10/29/15 6  
suggested that resonance alpha can be increased (reducing criticality) to compensate the lower PFNS average energy. Such change is supported by LANL Tovesson fission resonance data which is lower than Gwin. More resonance work is needed

# 239Pu data – Chatillon versus Chatillon+Granier-correction & Role of removing Staples data

- » Staples data suffer from unrecognized at the time large multiple scattering corrections



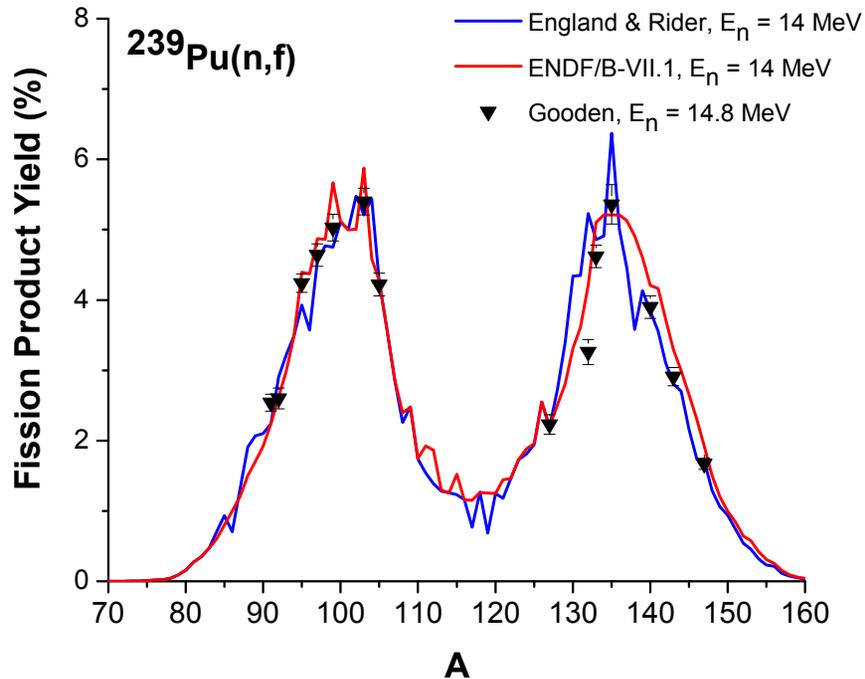
# Preliminary Results for $^{239}\text{Pu}$ . Although data appear to largely support VII.1, much work needed to integrate into a VIII Evaluation (resonances and high energy)



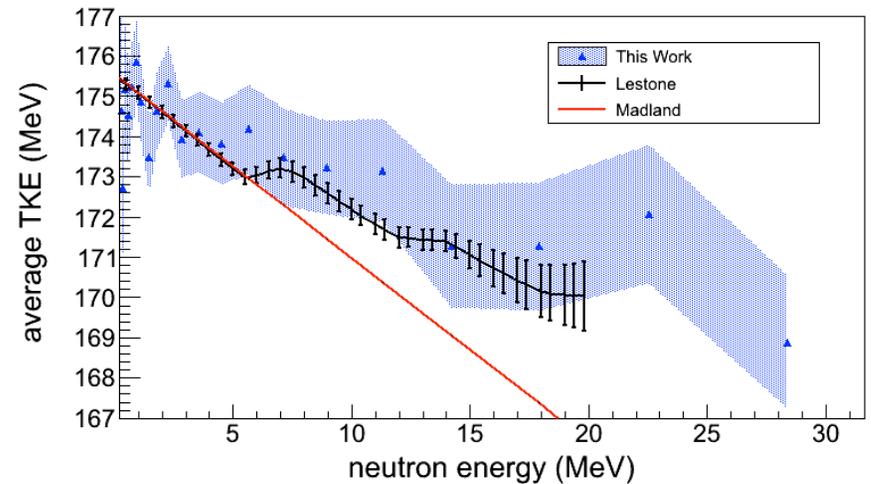
- **Issues in keV region analysis largely resolved**
- **Working through systematic uncertainties**

# 239Pu fission products

- » Update 14 MeV (and 0.5 MeV if needed) FPYs in ENDF, based on recent TUNL-LLNL-LANL Gooden *et al.* measurements



Some, but not all, VII.0->VII.1 changes supported by new data



First complete TKE measurement to above 14 MeV will influence a B-VIII fission energy change

## 56Fe pre-VIII file, NAME= beta1 (Svn rev.88)

- » **Major new 56Fe evaluation from BNL, see next talk by BNL:**
- » **Includes:**
  - » ORNL resonances up to 846 keV with JENDL-4.0 angular distributions
  - » total 846keV - 4 MeV: JEFF-3.2 (smoothed Berthold/Weigmann data)
  - » MT51,52 up to 4 MeV: smoothed Negret (Geel) data
  - » Remaining reactions EMPIRE calculations up to 29 MeV
    - » Gilbert-Cameron LD instead of microscopic HFB to improve neutron spectra
    - » R. Haight alpha emission reproduced, improved (n,2n), inelastic consistent with Nelson data after Chinese corrections
  - » RPI semi-integral data testing performed on beta0(!) version indicated need for improvement of neutron spectra and resonances (beta1 under testing)
  - » Preliminary validation comparable to VII.1 except 2 experiments
- » **Known Issues not yet addressed:**
  - » Decide on RR region (new ORNL evaluation?) and ang. distributions
  - » Extension to higher energies, covariances, other isotopes

# 16O pre-VIII file, NAME= o16 =5c IAEA\_halead (An updated version has recently been released by Hale)

» **Major new 16O evaluation from LANL, merged with VII.1 above ~6 MeV by IAEA**

» **Includes:**

» R-matrix leads to ~30% increased (n,a) in the 3-6 MeV range – closer to where B-VI.8 was before the B-VII reduction.

» Fair agreement with new RPI total cross section data in 3.2 – 6 MeV region (C/E = 1.01, VII.1 was 0.988).

» **Known Issues not yet addressed:**

» Data testing on transmission problem – issues identified.

» Doesn't quite match the Plompen et al CIELO thermal elastic/total recommendation (3.765 bars) – Gerry has reasons for this!

» Waiting for possible LANL LENZ (n,a) 3-5 MeV measurement relative to  ${}^6\text{Li}(n,a)$

» Merging new Hale evaluation with higher energy (>8 MeV) old data

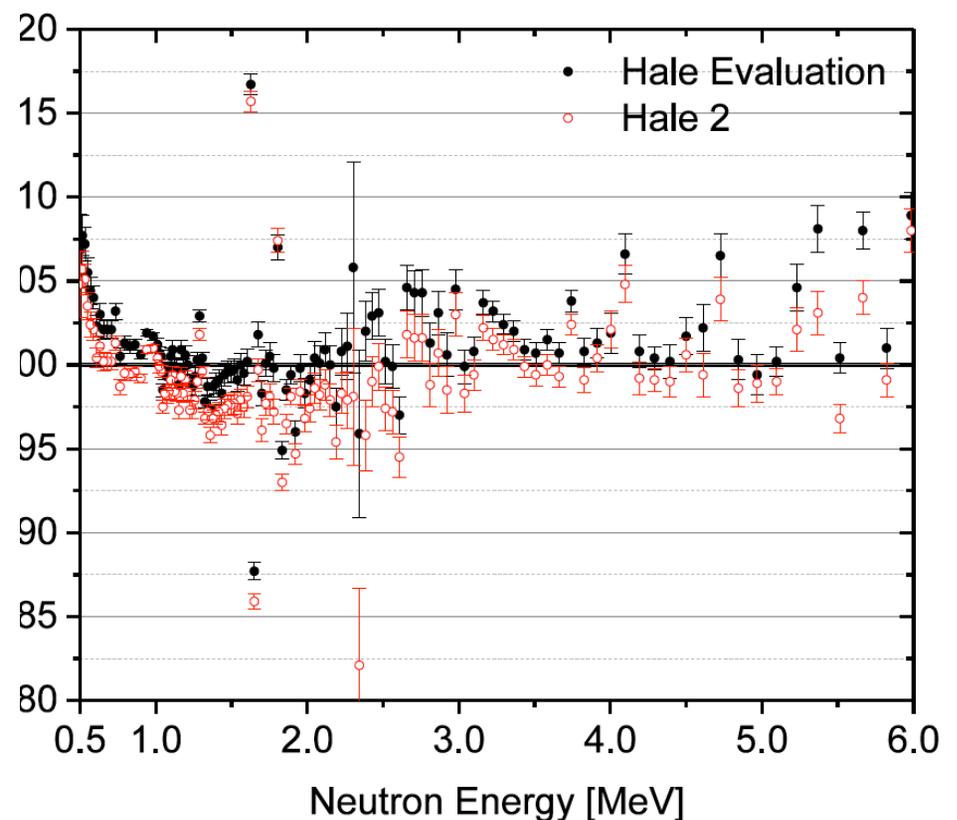
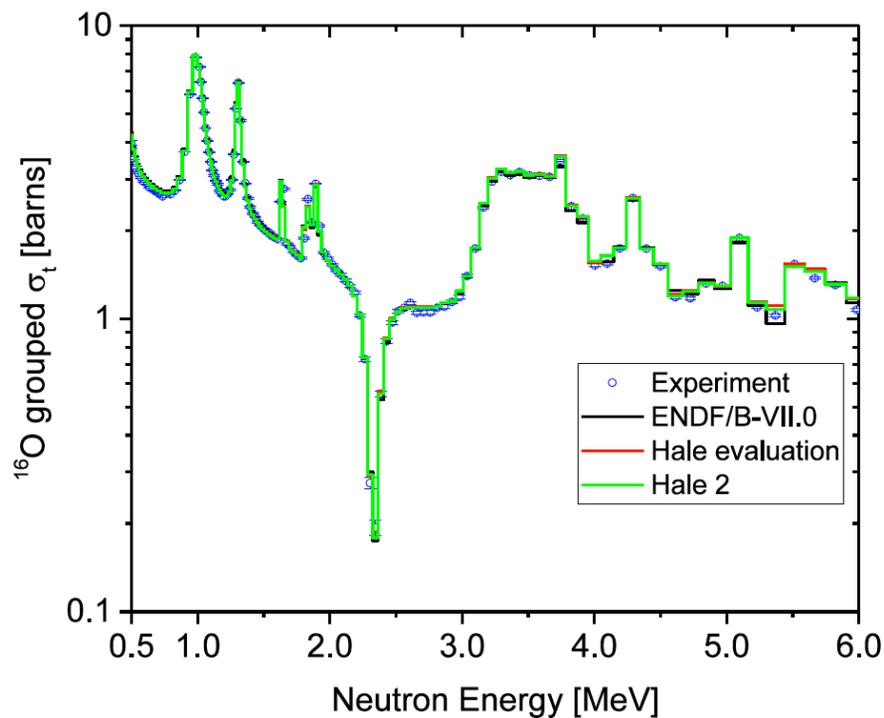
» Comparison with ORNL & Kunieda calcs? Details of work planned?

» Capture focus (Haxton/nucleosynthesis) esp. 10-20 keV (Igashira, Dubovichenko)

# 16O Hale evaluations compares well with new RPI data

- » Ratio of Integral from 3.2-6 MeV Hale=1.01 +/- 0.03; Hale2=1.005 +/- 0.003
- » In the 1-2 MeV Hale2's lower total cross section is influenced by other data

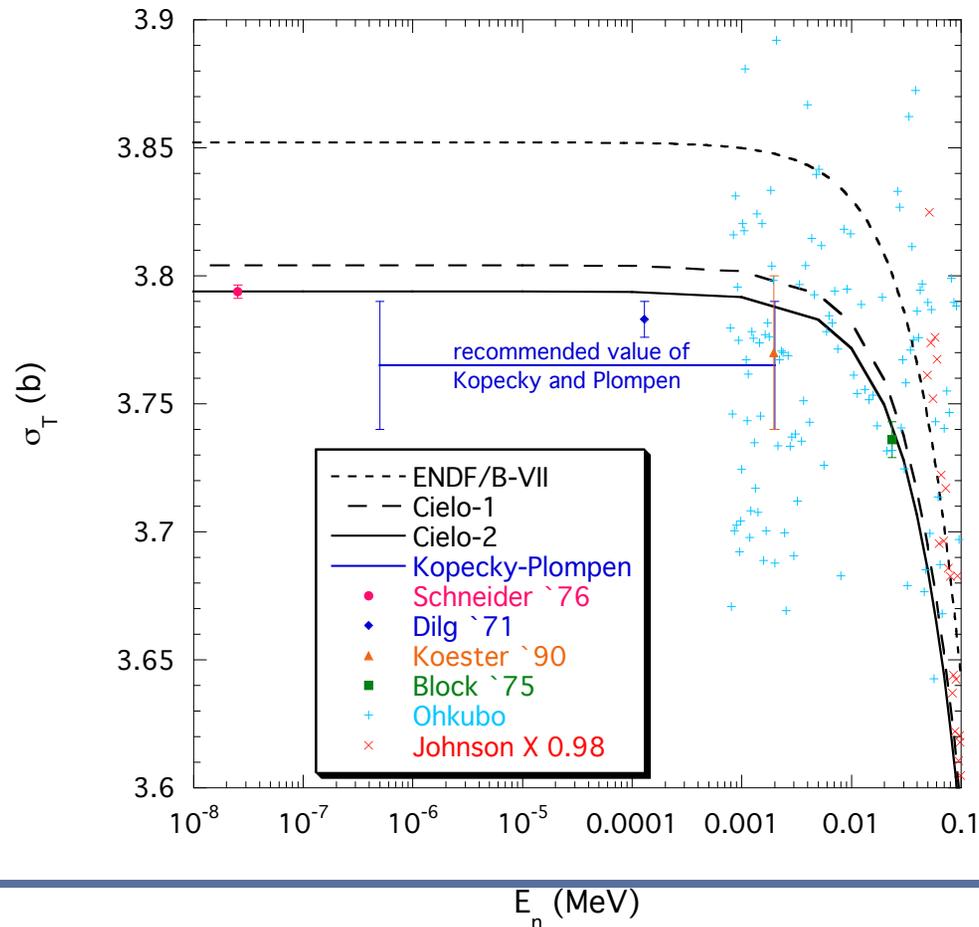
## C/E Ratios



# 16O Hale evaluations at low energies compared to CIELO work of Kopecky, Plompen, Lubitz, ...

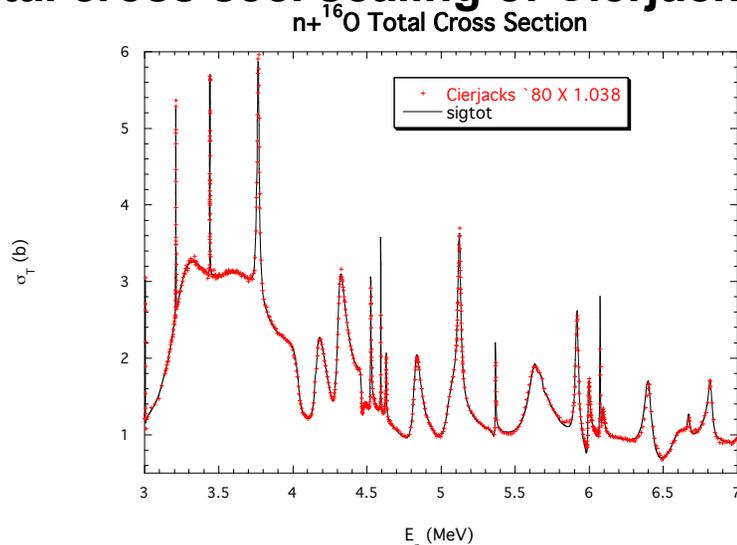
- » Slightly different from their 3.765 b. Resolve differences if possible. Schneider, with Ohkubo and Johnson, push for a value slightly higher than Kopeck et al's assessment. (Need to add Nistler, but unlikely to change assesment)

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

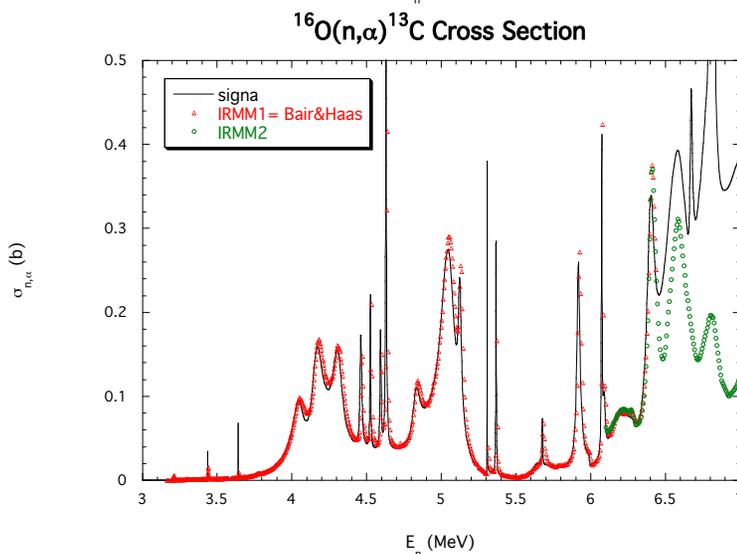
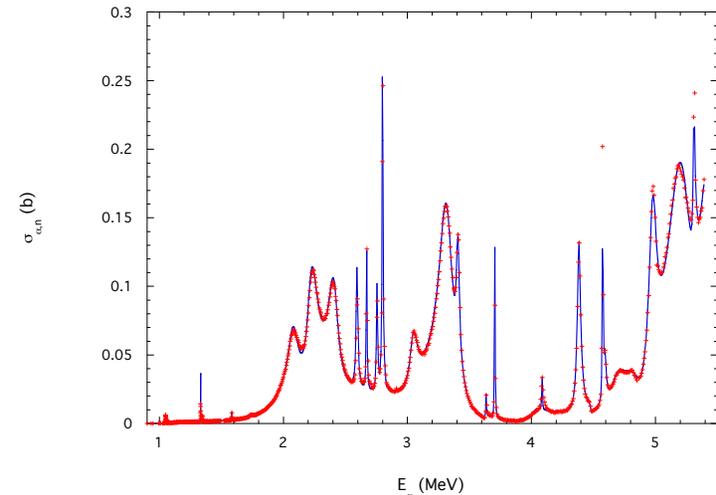


# 16O Hale evaluations for total cross section and n,alpha (New evaluation of a few weeks ago... but similar to tested iaea-halead file )

» **Total cross sec. scaling of Cierjacks consistent with other CIELO conclusions**



Inverse Bair-Haas data used in fit – Hale's  
R-matrix finds a solution  $\sim 6\%$  lower  
<sup>13</sup>C( $\alpha$ ,n)<sup>16</sup>O Cross Section

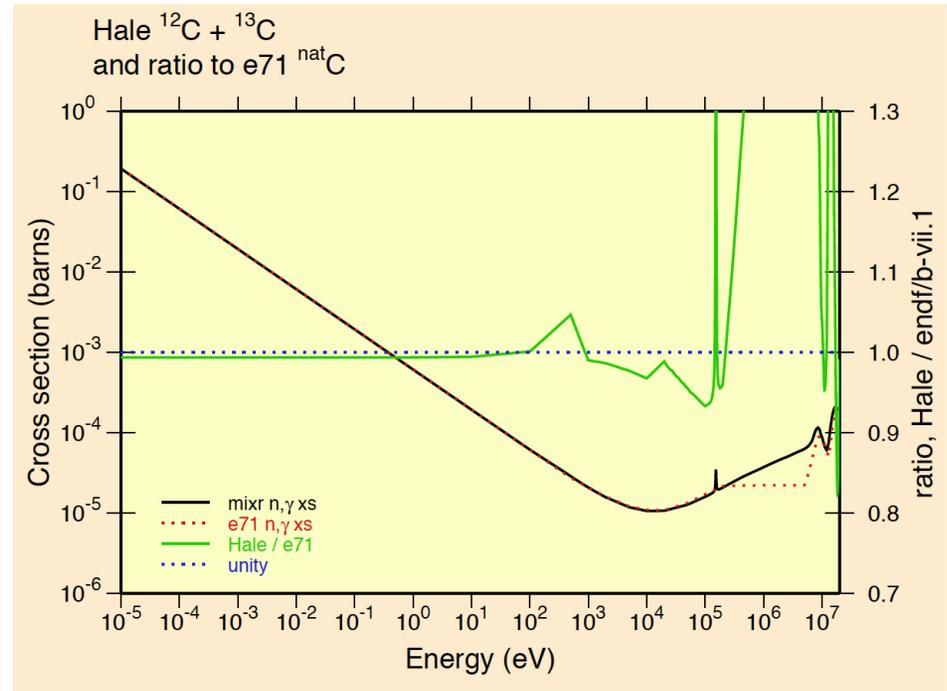
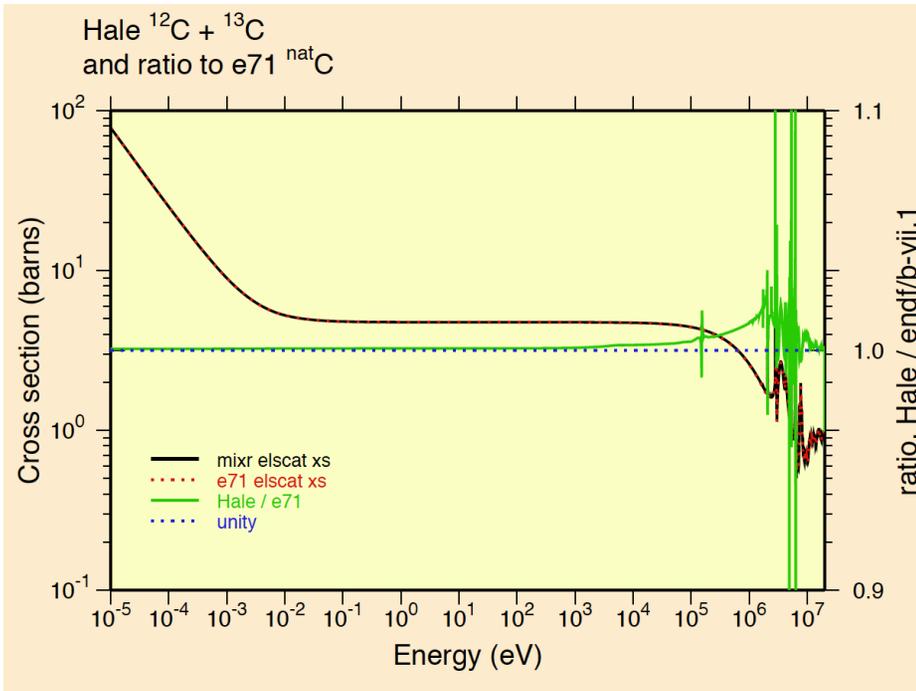


**IRMM1 is Bair-Haas converted to  
inverse channel, with no  
renormalization (as recommended  
by Giorganis).**

[earlier IRMM Giorganis had the 4.2 MeV peak  
near just over 0.1b, more like old VII.1, before  
he recommended a higher normalization]

Differences above 6.5 MeV are due to LANL R-  
matrix fit influenced by total cross section  
data (unitarity) and Bair-Haas inverse data

# 12C and 13C. Hale has test evaluations for replacing natC in ENDF. Care must be taken owing to 12C(n,n') elastic scattering as a standard



Ratio to Standard exceed 1-1.5% in the 1-2 MeV range, beyond the 0.68% standard uncertainty

Kahler has check performance of LCT-060, Russian RBMK reactor, given impact of VII.0->VII.1 change.

# Conclusions

**Much progress, with improved physics**

**We have a base set of files that perform adequately in integral simulations**

- future improvements in integral performance still a goal

**Much work will be also needed to add credible covariances**

**This creates optimism that we can release ENDF/B-VIII in the 2017/2018 time frame**

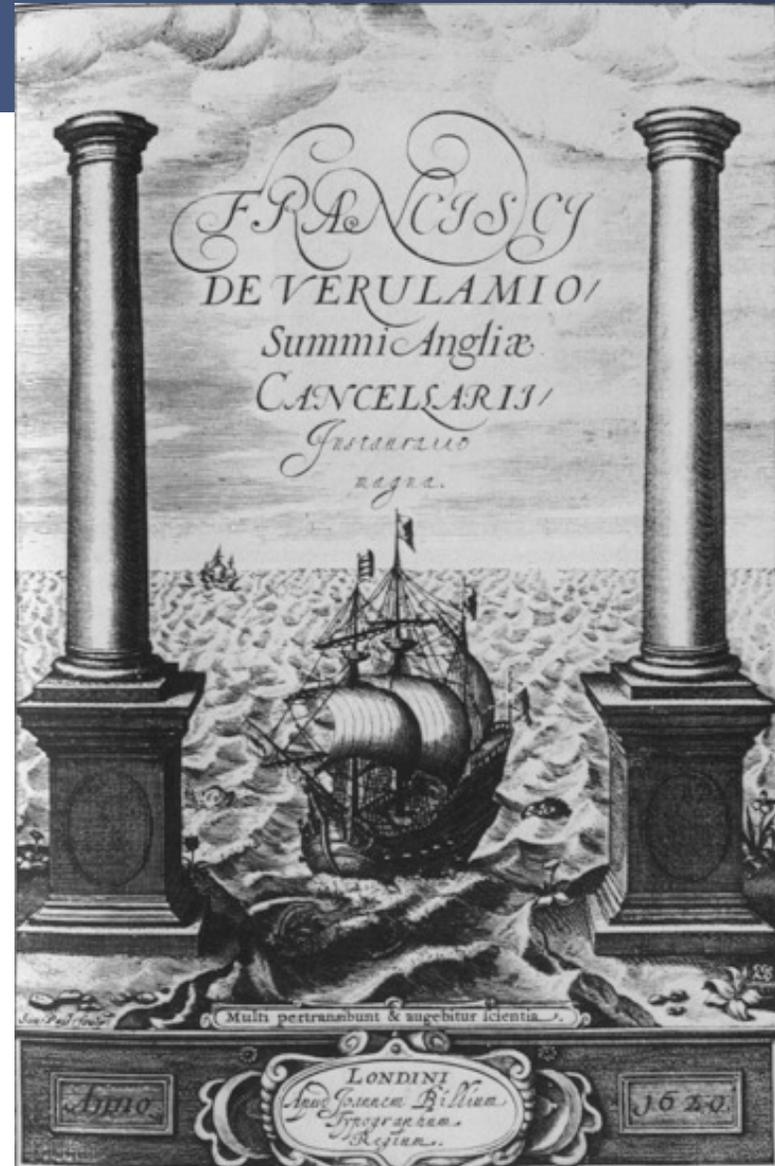
- NDS big paper for CIELO & VIII planned for Jan 2018
- This would imply we release in Nov 2017, 2 years from now
- Implies most essential nuclides frozen ~ 1 year away

# Nuclear never ends ...

**Plus Ultra** : there is more beyond  
(motto of the great scientific  
pioneers of the 16<sup>th</sup> & 17<sup>th</sup>  
Century)

Francis Bacon's *Novum Organum*  
(1620): Straits of Gibraltar  
flanked by the colossal pillars  
of Hercules.

Inscription: Many shall pass too  
and fro and knowledge shall  
be increased



# Plan for Reaching ENDF/B-VIII Release in 2018

## Higher risk:

- Inelastic scattering
- Capture in fast region
- More PFNS upgrades
- ...

END/B-VIII.0 2017/18  
- Further major upgrades

## Pre-ENDF/B-VIII, 2015

- Base upgrades established (covariances not yet added)
- + numerous variants
- 1H, 16O, 56Fe, 235,8U, 239Pu,
- 9Be?, C, Ne, Ca, Ni, Cu, As, Re, W, ...
- Thermal kernels (SG42)

END/B-VIII.0 2017/18  
- Modest upgrades

CIELO help

## Labs providing evaluations:

- LANL, ORNL, BNL
- IAEA, IRSN, CEA, IRMM
- CAB, CNL

## Low risk:

- Fission product yields, TKE
- PFGS (fission gammas)
- PFNU (nu)
- ...

END/B-VII.1, 2011  
- Widely used in DOE & around world