
Mark Chadwick,
LANL

WPEC-SG40 (CIELO), Paris, May17, 2017

International CIELO Collaboration

Experiments:

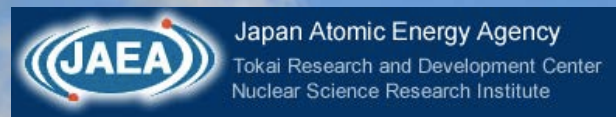
Some of the many experimental facilities that measured new data supporting CIELO

Reduced US capability in nuclear science led to creation of international collab. Via

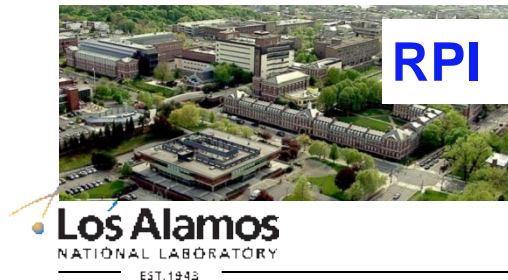
Nuclear Energy Agency (Paris) & IAEA



JRC/Geel, Belgium



LANL/LANSCE CEA

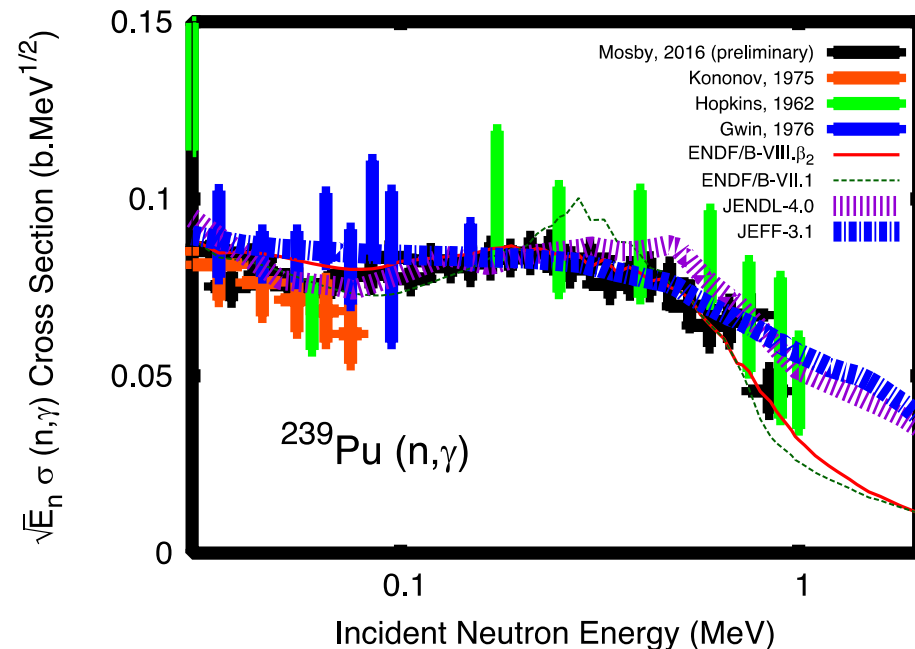


Plutonium-239

Updates:

- Uses new Standards fission
- Adopted NEA/WPEC Subgroup34 resonance analysis (CEA-ORNL), with IAEA mods to unresolved to match standards fission
- New capture data from LANL/DANCE by Mosby, Jandel, et al., used > 30 keV
- PFNS >5 MeV from Neudecker
 - Existing evaluation matches LANL NUEX data, & Chatillon's CEA data
 - we await LANSCE "Chi-nu" exp. data
- Future work will be an updated resonance analysis, (& extension to 4 keV), and theoretical treatment of capture by Kawano *et al.* including the M1 scissors mode; inelastics

New DANCE data has now been used, from 30 keV to 100s of keV in CIELO-1



Prompt fission neutron spectra (PFNS) from IAEA CRP (IAEA at thermal; Talou-Rising & Neudecker at higher energies)

Average energy of PFNS

For 1.5 MeV incident energy,
ratio of ^{239}Pu to ^{235}U spectrum

II - open symbols
ENDF/B-VIII.0 β_2 - full symbols

Lestone & Shores, LANL

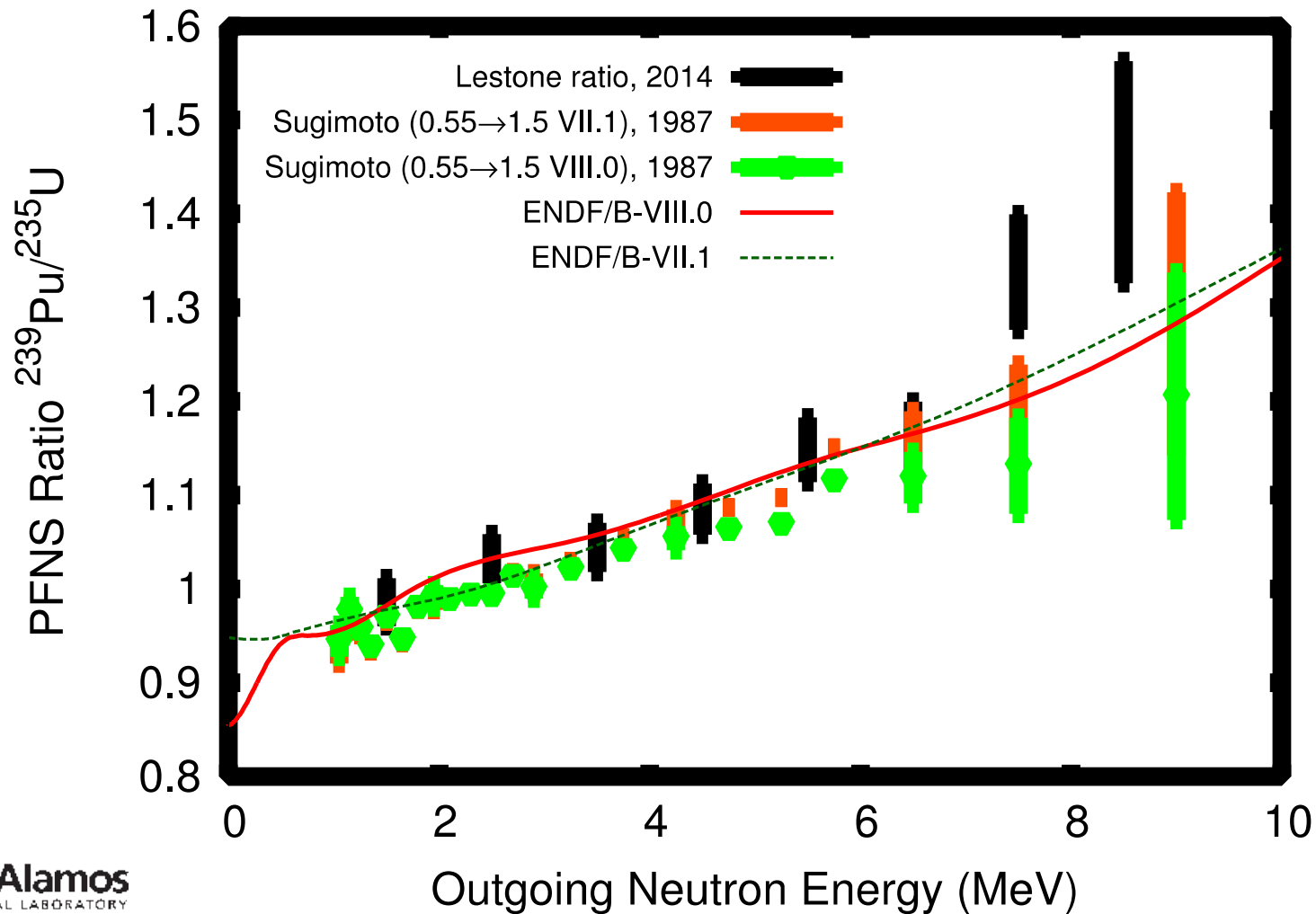
Sugimoto (0.55 \rightarrow 1.5 MeV, B-VIII.0 β_2)

Plutonium is harder

Thermal PFNS average energy now 2.00 MeV. This lower average energy increases the reactivity of uranium thermal crits.

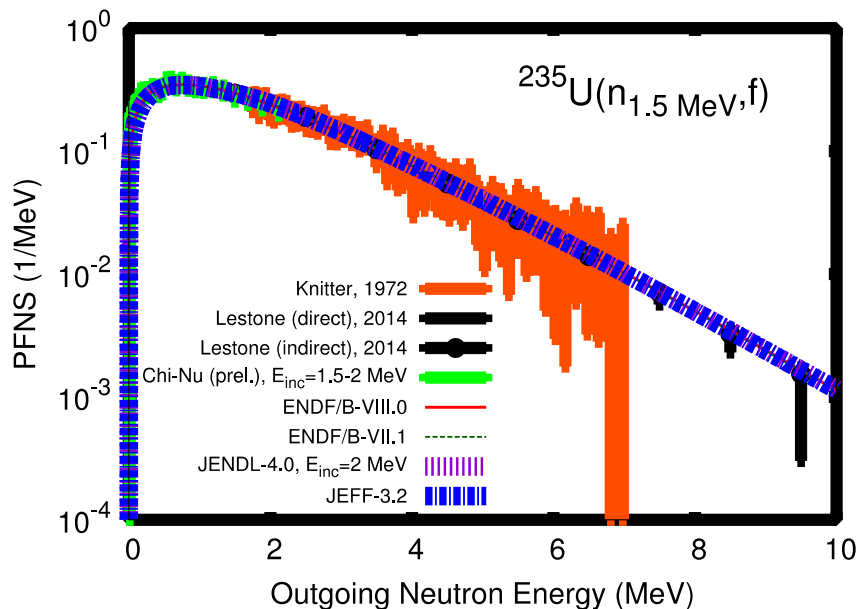
Like Watt (PRC, 1952), Los Alamos (also 2.00 MeV)

Prompt fission spectrum – ^{239}Pu is hotter than ^{235}U



Prompt Pu fission spectrum — waiting for Chi-nu ^{239}Pu data.

Here is what we got for ^{235}U
from Chi-nu/LANSCE



Note how very sensitive our applications are to PFNS...

Even though we do not have new ^{239}Pu Chi-nu data, we made a trial ENDF-8 file using a slightly softer PFNS, as was the case for ^{235}U .

But our applications are very sensitive to this change. We withdrew this file, pending getting the data

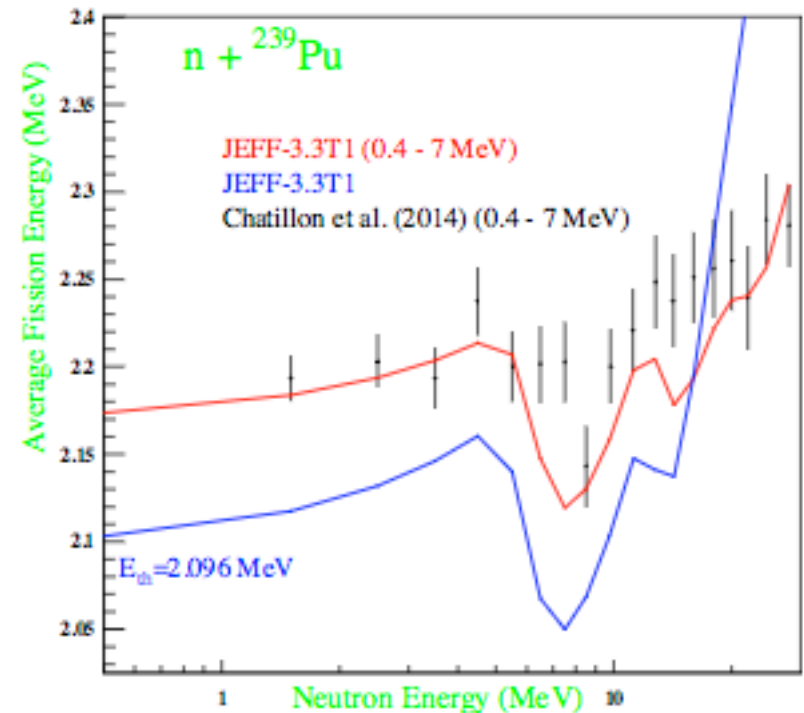
Pu239; Example of CEA/Bll work in CIELO-2

^{235}U , ^{238}U and ^{239}Pu JEFF-3.3T1 evaluation

Completely new evaluations

- New FILE 2,
- New softer prompt fission neutron spectra, with new prompt neutron multiplicity,
- New OMP parameters,
- New elastic and inelastic cross sections,
- Fission cross section from IAEA standards, but close to the BRC model calculations.
- Covariances (COMAC or T6).

^{239}Pu



We also use common models to track progress

We routinely calculate 1000s of critical assembly k_{eff} that span

- fast, intermediate, thermal energies
- metals, compounds
- various SNMs (Pu, HEU, LEU, U-233, Np, ...)

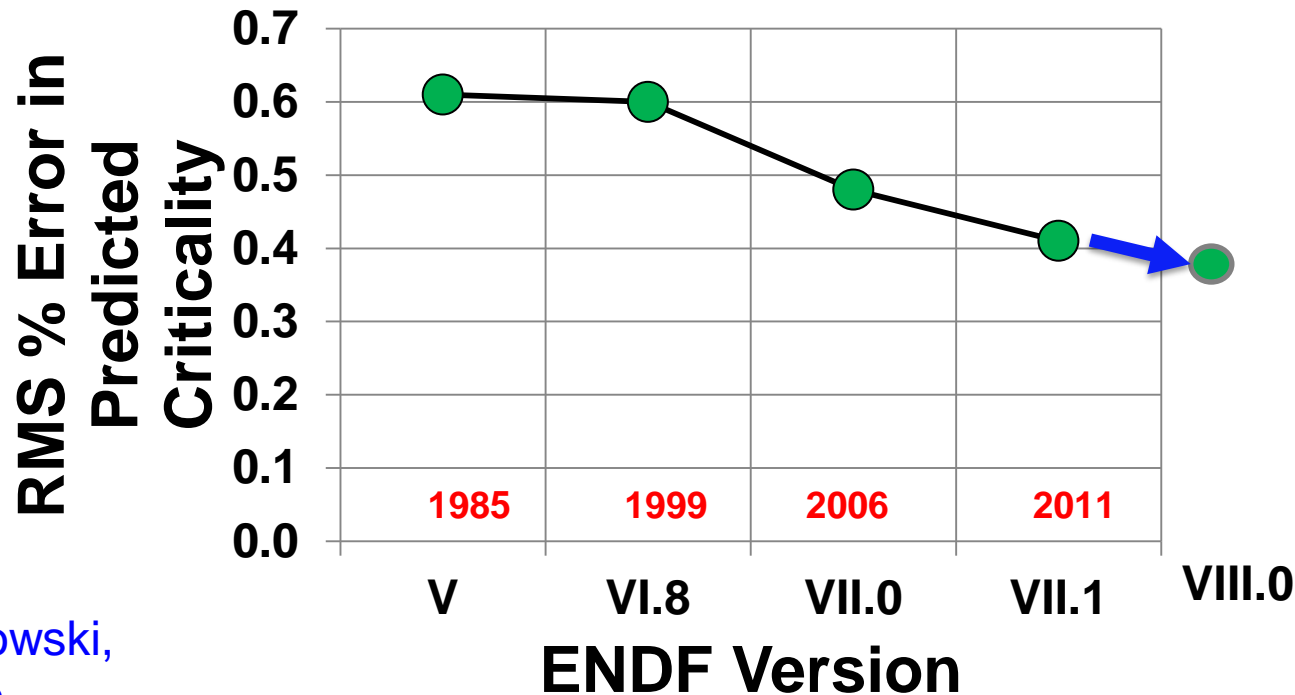
with the same physical data & methods

- same database, e.g. ENDF/B-VIII.0-beta4
- same NJOY processing, & transport code MCNP6

e.g. “Mosteller validation suite” of 119 critical assemblies that we

Where did we end, for ENDF/B-VIII CIELO files?

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

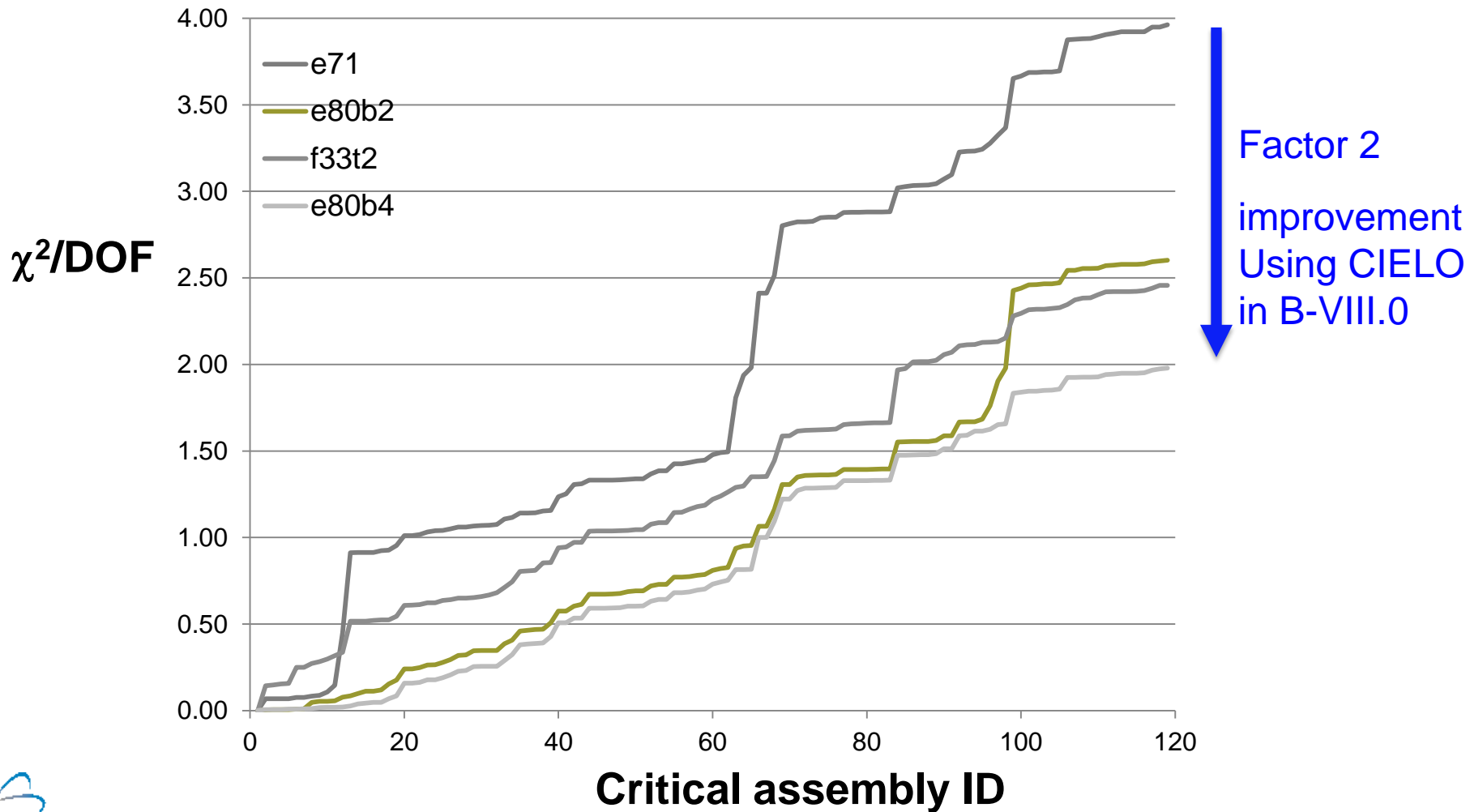


Kiedrowski,
Brown,
Trkov

But better underlying physics, &
 χ^2/DOF has been reduced from 3.9 to 1.96

0.4% k_{eff} matters!
Causes ...

Chi-2 reduction with CIELO files in ENDF/B-VIII



Some highlights of integral data testing & performance

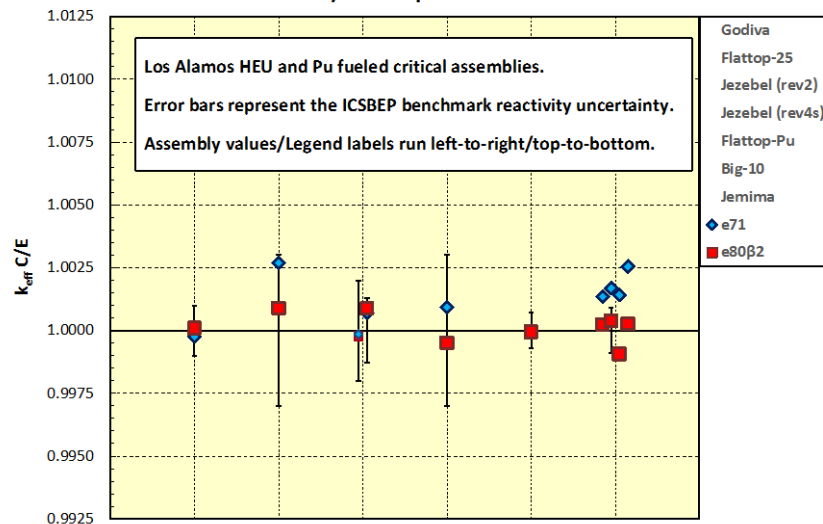
Fast reactor sodium void reactivity worth

Benchmark tests of ENDF/B-VIII.0 beta1
using sodium void reactivity worth of FCA-XXVII-1 assembly

M. Fukushima, K. Yokoyama, O. Iwamoto, T. Jin, and Y. Nagaya
Japan Atomic Energy Agency
July 2016

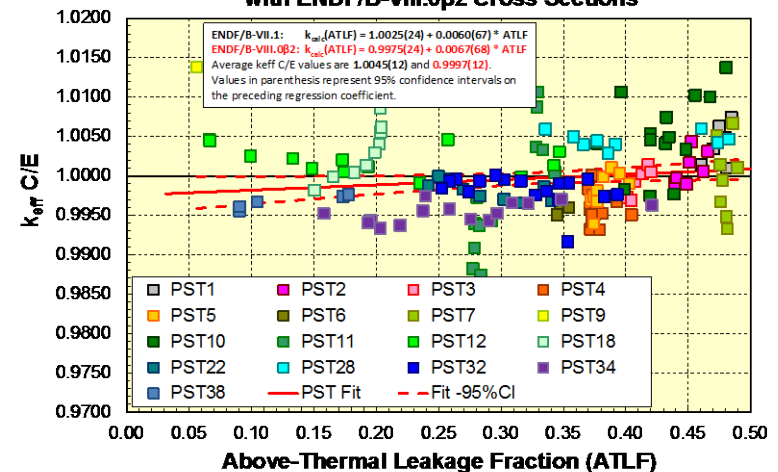
Fast crits perform well still

Calculated Eigenvalues with ENDF/B-VII.1
and ENDF/B-VIII.0 β 2 Cross Sections



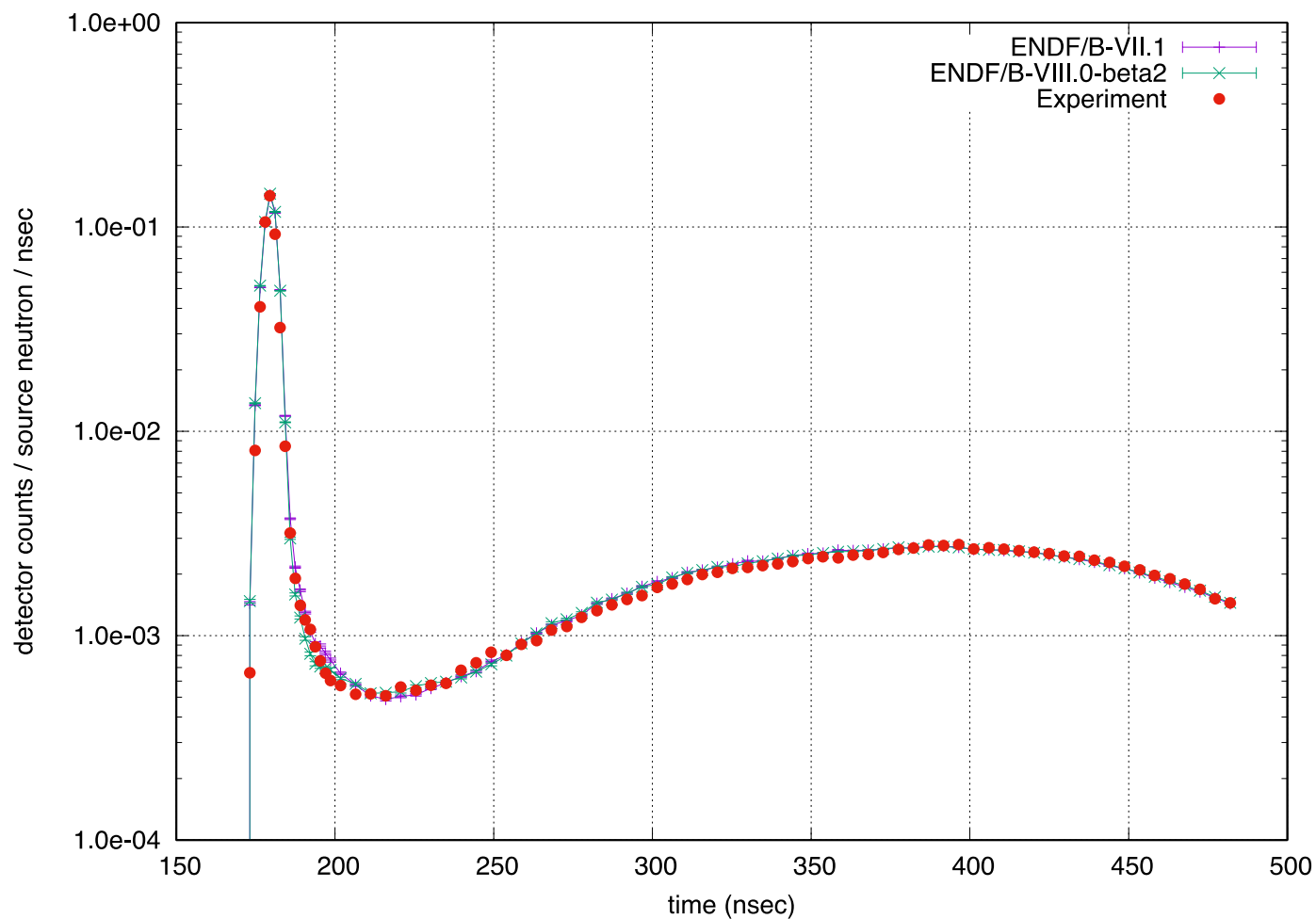
Plutonium solutions now predicted much better

Calculated Pu-SOL-THERM Eigenvalues
with ENDF/B-VIII.0 β 2 Cross Sections

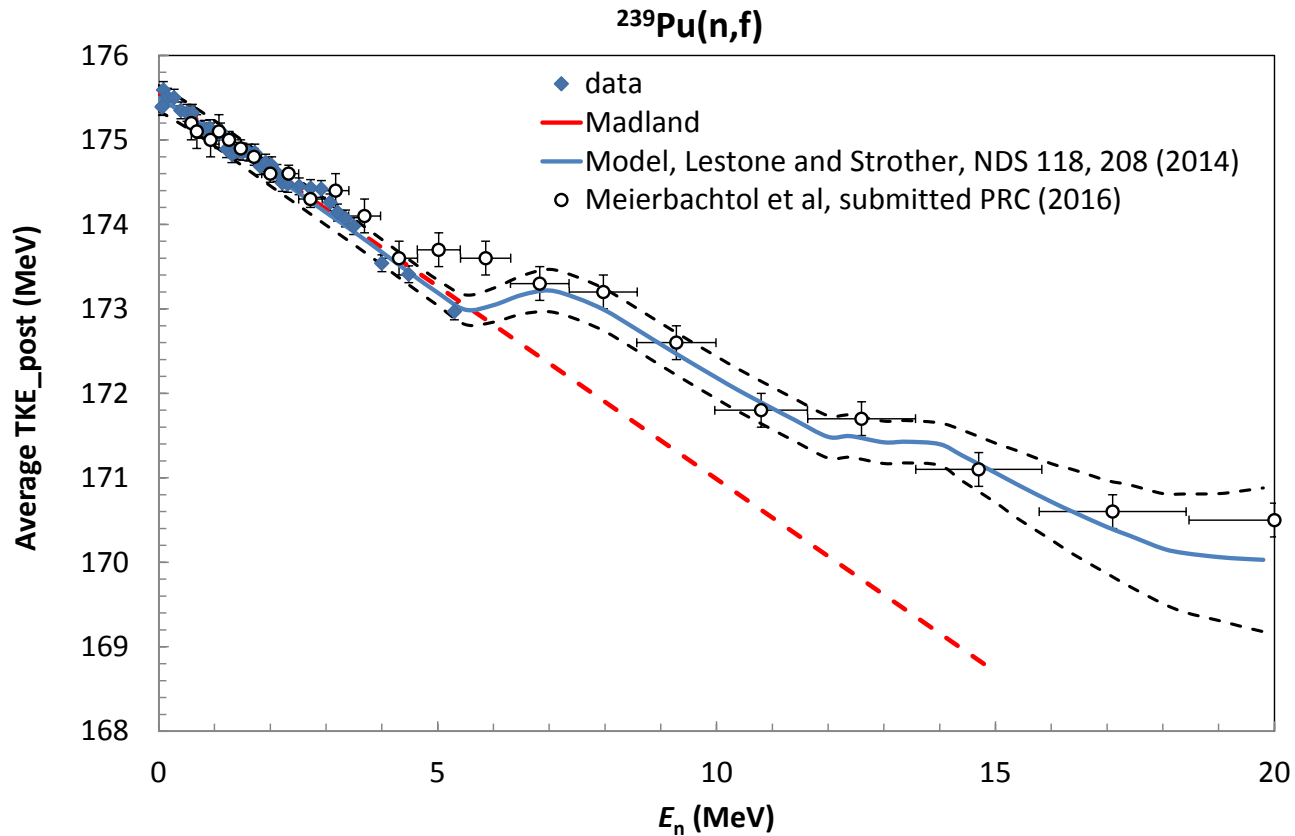


Kahler, Trkov, Fukushima

Livermore pulsed sphere

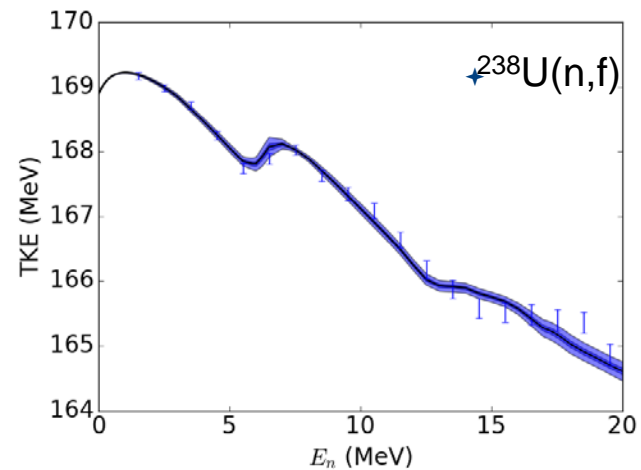
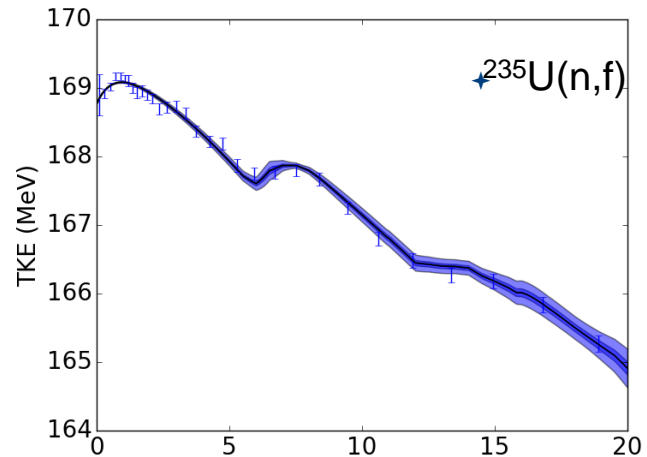
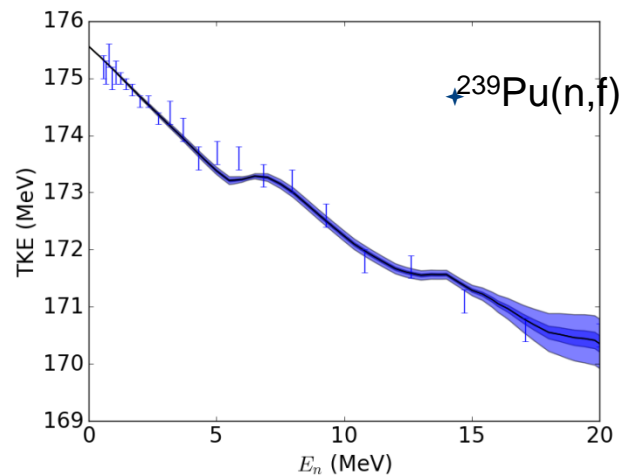


Fission energy release TKE is being updated, based on new LANSCE data and Lestone model calculations

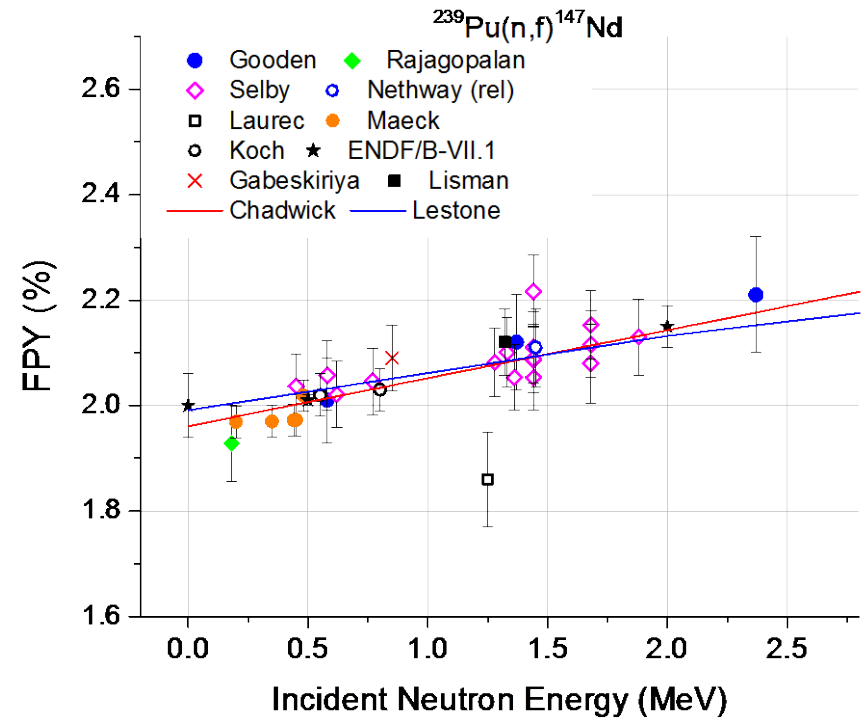
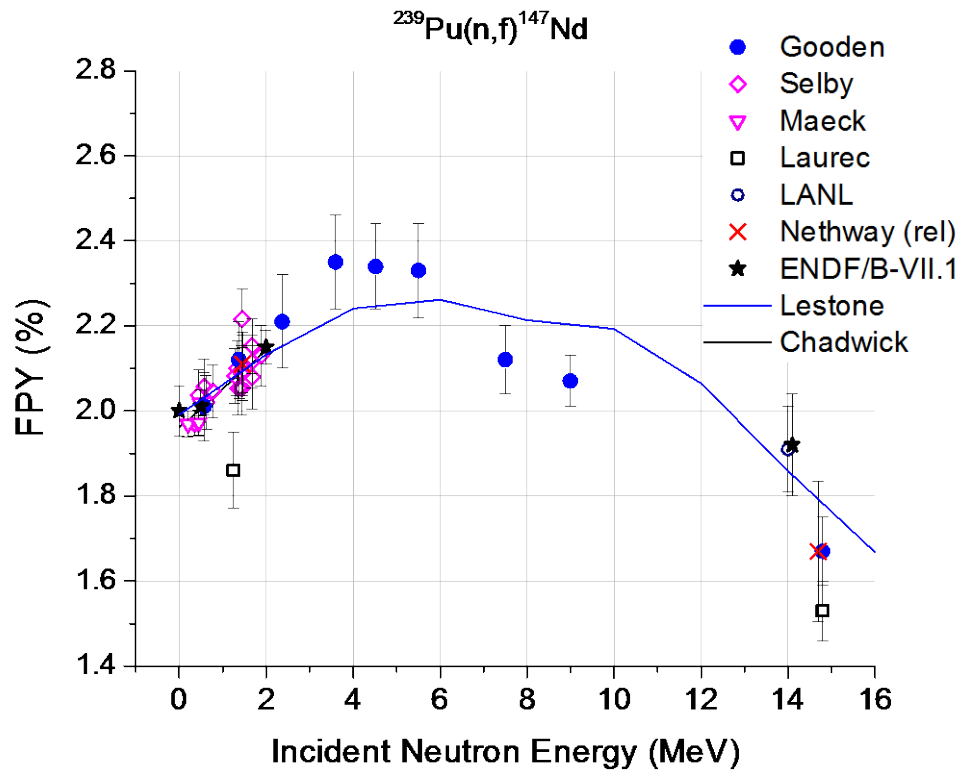


TKE versus incident neutron energy going into ENDF-VIII for other actinides

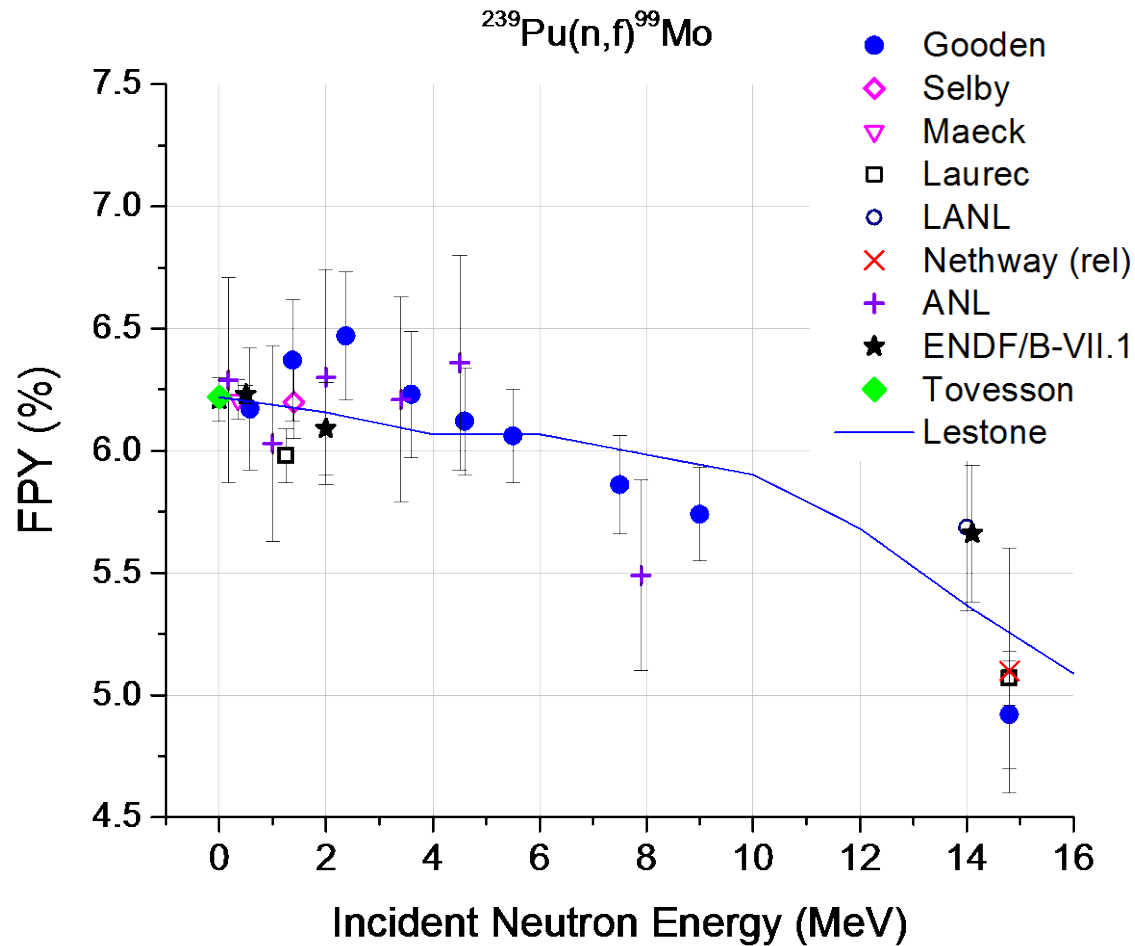
Model used to make predictions in 2014 has now been used as a tool to evaluate data recently measured at LANSCE.



Fission product yields



Fission product yields



PFGS puzzle we are now studying

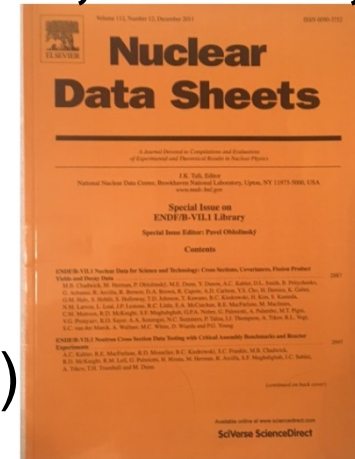
Frehaut (CEA) PFGS total energy and
Drake (LANL) total gamma production
energy seem inconsistent

ENDF – evolution over the years



Maintained at Brookhaven (Brown, Herman, Sonzogni)

- evaluations (Chadwick)
- validation (Kahler, Trkov)
- formats (Dunn); cov (Smith)
- experiment (Danon)



ENDF/B-VI

1990

ENDF/B-VII.1

2006

Major upgrades

LANL2006
database

ENDF/B-VII.1

2011

Upgrades just to:

- covariances
- minor actinides
- structurals

ENDF/B-VIII

2017

Major upgrades to:

- standards
- actinides
- TN reactions
- structurals

CIELO



Operated by Los Alamos National Security, LLC for NNSA

LANL ENDF8 talk, April 6, 2017



Some of the great scientists who led earlier evaluations (only retirees shown)

Shibata-san



Cecil Lubitz



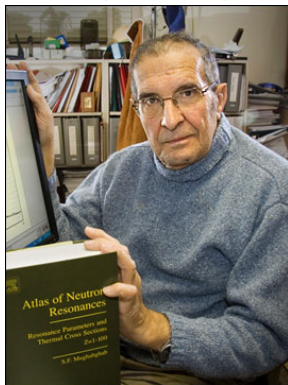
Herve Derrien



Herbert Vonach



Said Mughabghab



Nancy Larson



Phil Young



Jacques Raynal



CIELO: Lessons Learned

We accomplished an expedited advance in evaluation file capabilities, by:

- *broad collaboration & enthusiasm*
- *significant resource investments by participants, in time and \$*
- *but progress was still slow!*

We demonstrated it is possible to adopt standards, without adjustment away from standards (with a couple of exceptions)

- *not easy; expanded computational tools in future may make this easier*
- *previous small standards uncertainties seem to be correct – new standards cross sections used in CIELO are within 2 sigmas*

In many cases, the previous perceived “too large uncertainties” were correct, e.g. $^{235}\text{U}(n,\gamma)$, where data changed by 15-40%

A major challenge – and accomplishment – was developing a suite of CIELO evaluations that perform well in concert, as a suite

CIELO: Outstanding problems that need future work

More integral validation testing

Complete covariances, and assess their quality

^{16}O : although much more consensus was reached, some still argue for a lower (n, α) as in previous evaluations. Experiments needed to resolve this

^{235}U : nubar needs more constraints. PFNS still under-constrained. Capture data in the 10s-100s keV region need validating.

^{238}U : LCT solutions now slightly under-predicted... PFNS still under-constrained.

^{239}Pu : New resonance analysis would be valuable, upgrading SG34 and taking advantage of recent fission & capture data. Inelastic scattering in the keV-MeV region – needs a modern analysis. PFNS still under-constrained.

CIELO: Suggested path forward, to maintain momentum

Nuclear Energy Agency/WPEC coordinated efforts

- Focus next phase on collaboration of CIELO evaluators with validation experts
- Focus on covariance data assessments
- Take advantage of NEA staff sensitivity tools and capabilities

IAEA Nuclear Data Section

- Focus on CIELO cross section improvements
- Continued coordination with standards
- Take advantage of IAEA staff reaction code and evaluation capabilities

CIELO: Lessons Learned & Future Directions

Closer international collaboration is worthwhile, but many evaluators understandably want to maintain independent efforts

Much work still needed for resolving open questions

- exp. measurements are coming ...
- use of theory, UQ/sensitivity & simulation codes; future and covariance and validation testing needed

We demonstrated it is possible to adopt standards, without adjustment (with a couple of exceptions)

Project ends in 2017; follow-on being discussed with IAEA & NEA

Documenting CIELO work

- ⑩ *Set of papers for January NDS2018, edited by Oblozinsky*
- ⑩ *Papers on O, Fe, Actinides, Standards, PFNS, Capture, and a Main Summary paper (an evolution of our ND2016 proceedings paper):*

The CIELO Collaboration: Progress in International Evaluations of Neutron Reactions on Oxygen, Iron, Uranium and Plutonium

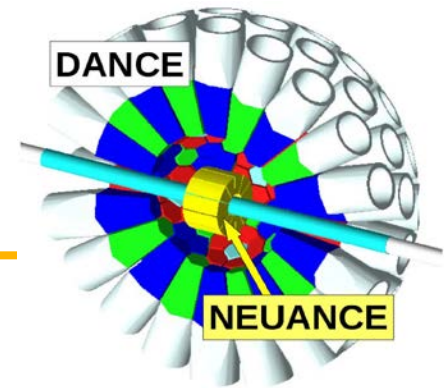
M.B. Chadwick^{1,*}, R. Capote², A. Trkov², A.C. Kahler¹, M.W. Herman³, D.A. Brown³, G.M. Hale¹, M. Pigni⁴, M. Dunn⁴, L. Leal⁵, A. Plompen⁶, P. Schillebeeck⁶, F.-J. Hambsch⁶, T. Kawano¹, P. Talou¹, M. Jandel¹, S. Mosby¹, J. Lestone¹, D. Neudecker¹, M. Rising¹, M. Paris¹, G.P.A. Nobre³, R. Arcilla³, S. Kopecky⁶, G. Giorginis⁶, O. Cabellos⁷, I. Hill⁷, E. Dupont⁷, Y. Danon⁸, Q. Jing⁹, G. Zhigang⁹, L. Tingjin⁹, L. Hanlin¹⁰, R. Xichao¹⁰, W. Haicheng¹⁰, M. Sin¹¹, E. Bauge¹², P. Romain¹², B. Morillon¹², G. Noguere¹³, R. Jacqmin¹³, O. Bouland¹³, C. De Saint Jean¹³, V.G. Pronyaev¹⁴, A. Ignatyuk¹⁴, K. Yokoyama¹⁵, M. Ishikawa¹⁵, T. Fukahori¹⁵, N. Iwamoto¹⁵, O. Iwamoto¹⁵, S. Kuneada¹⁵, C.R. Lubitz¹⁶, G. Palmiotti¹⁷, M Salvatores¹⁷, I. Kodeli¹⁸, B. Kiedrowski¹⁹, D. Roubtsov²⁰, I. Thompson²¹, S. Quaglion²¹, H.I. Kim²², Y.O. Lee²², A.J. Koning², A. Carlson²³, U. Fischer²⁴, and I. Sirakov²⁵

Backup

Future beyond O, Fe, U, Pu

⑩ *Next ?* :D,Li,Be,B,C,Na,Cr,Ni,Mo,^{240,241}Pu,²⁴¹Am

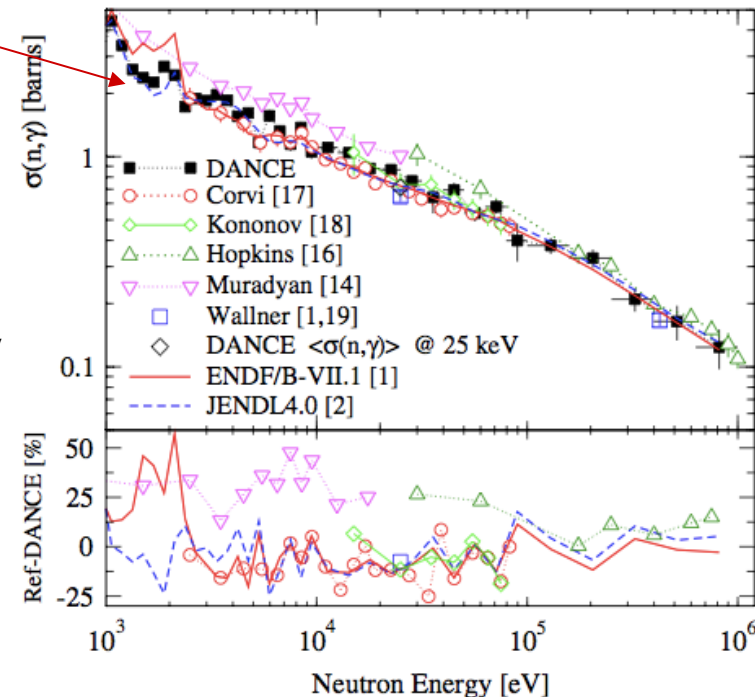
Uranium-235



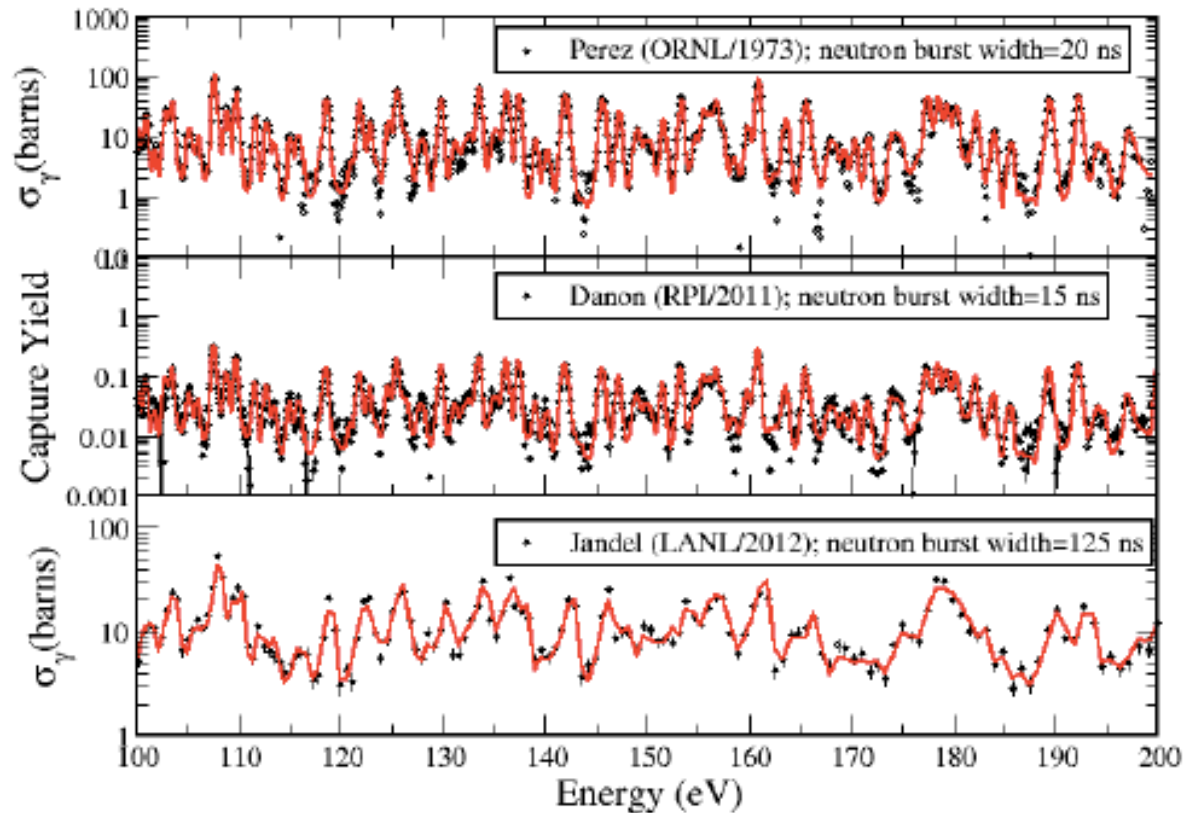
Challenge: How to maintain good integral performance while accommodating some large changes:

- Prompt PFNS (2.03 -> 2.00 MeV average energy @ thermal)
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Jandel's DANCE data has now been used up to 50 keV in CIELO-2



Foundational SAMMY resonance analysis by Leal *et al.*



Paper @ ND2016



Figure 5 : SAMMY fitting of the fission cross section in the 100 eV to 400 eV energy range.

Prompt fission neutron spectra (PFNS) from IAEA CRP (IAEA at thermal; Talou-Rising & Neudecker at higher energies)

Average energy of PFNS

For 1.5 MeV incident energy,
ratio of ^{239}Pu to ^{235}U spectrum

II - open symbols
ENDF/B-VIII.0 β_2 - full symbols

Lestone & Shores, LANL

Sugimoto (0.55 \rightarrow 1.5 MeV, B-VIII.0 β_2)

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Like Watt (PRC, 1952), Los Alamos (also 2.00 MeV)

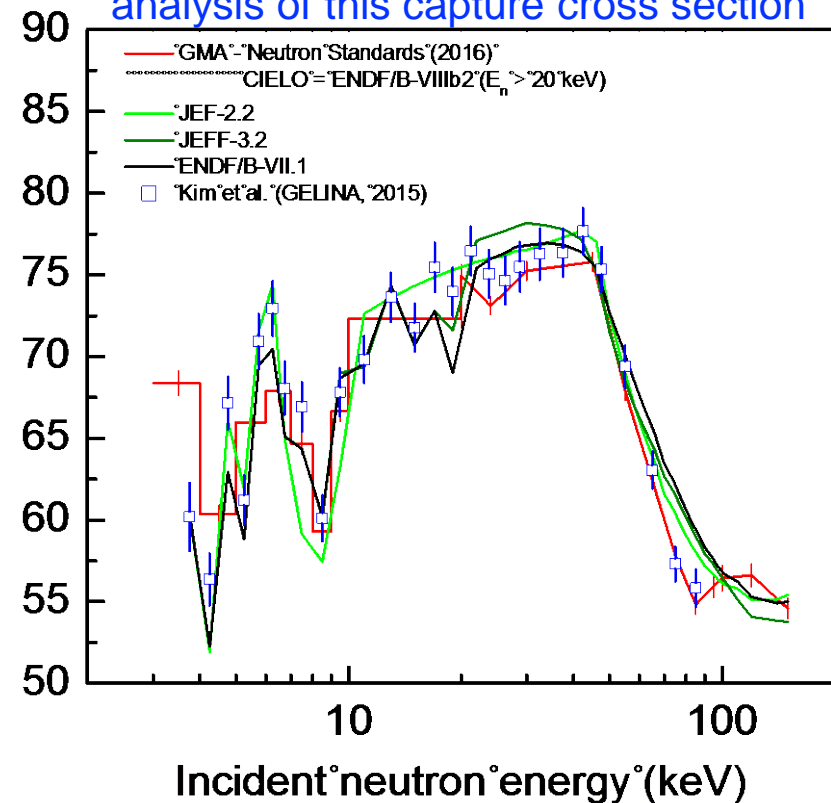
Uranium-238

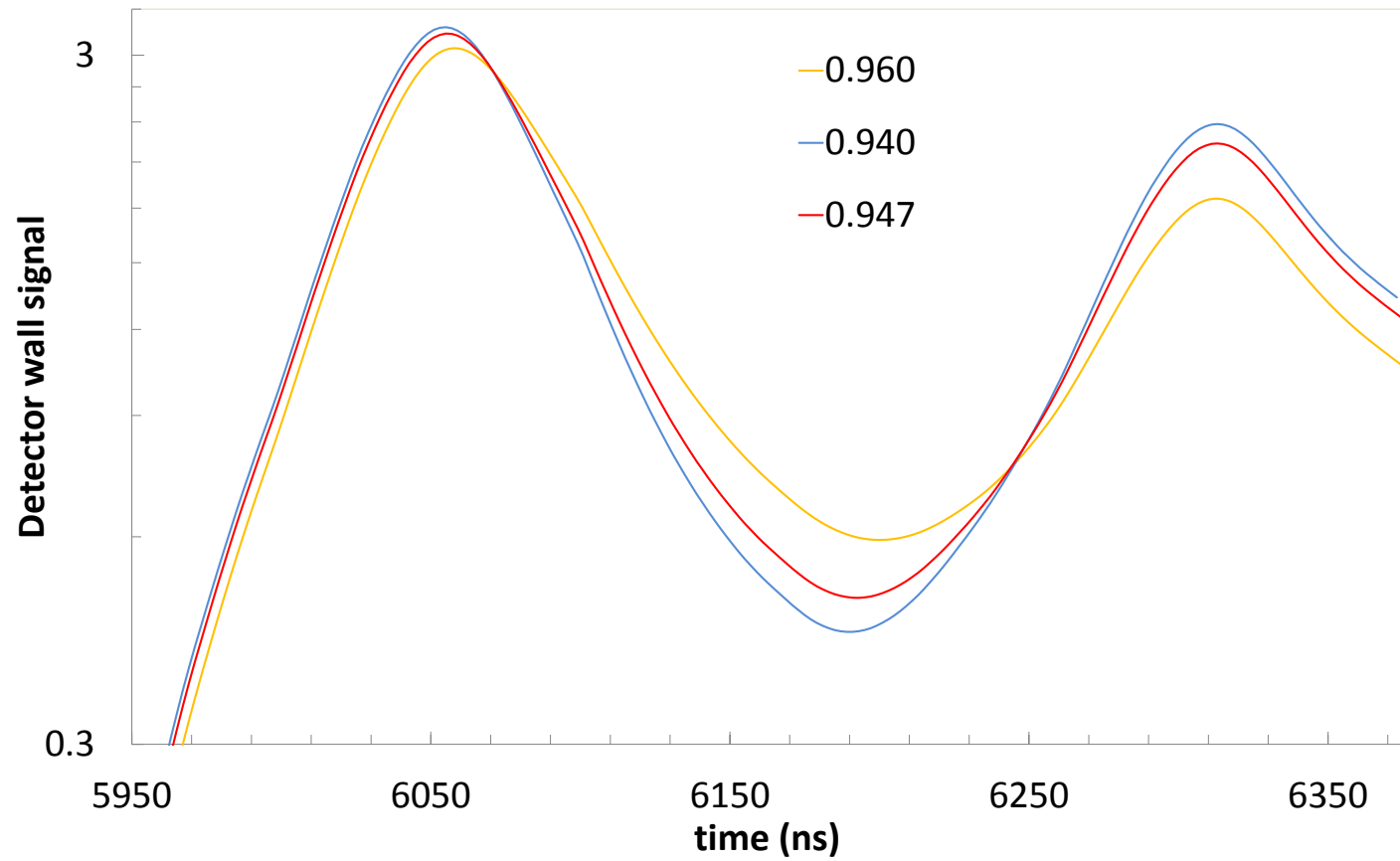
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$[\sigma \times E^{1/2}]^{oo} (b \cdot eV^{1/2})$

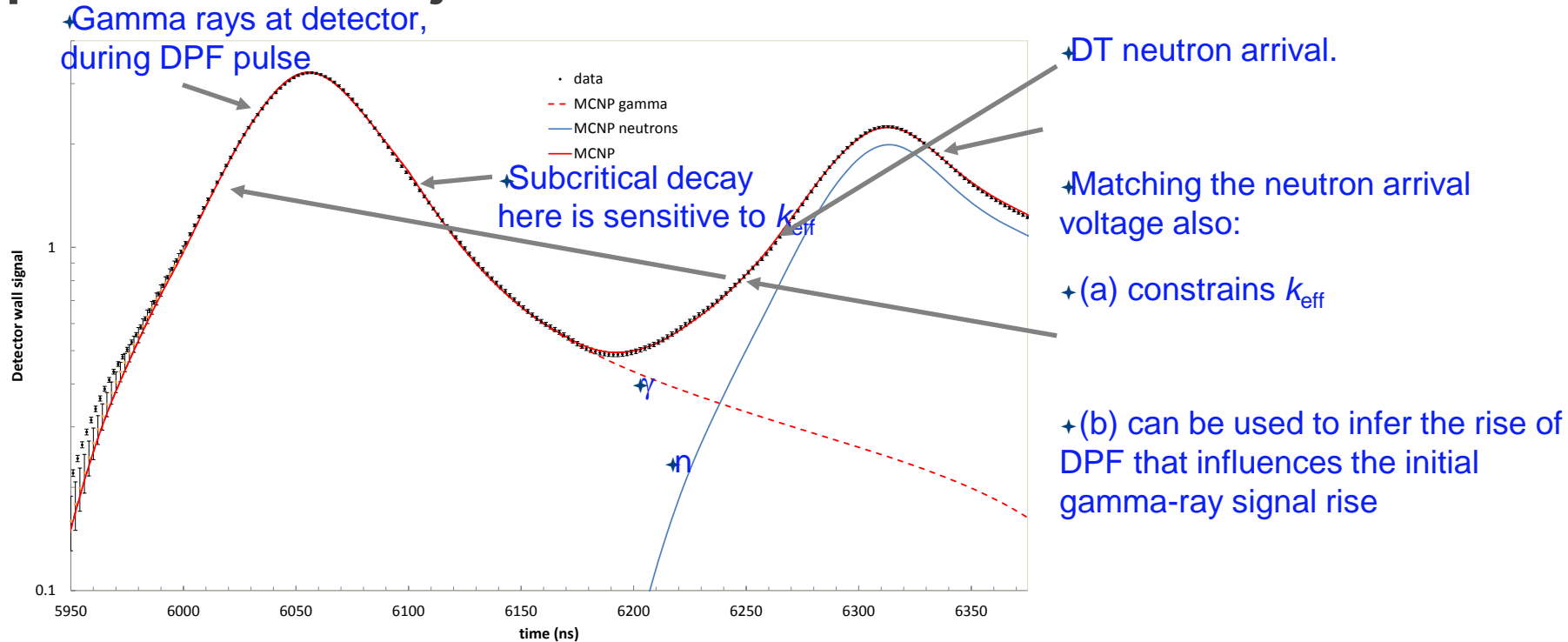
CIELO-1 uses the new standards analysis of this capture cross section





MCNP simulations of 13 DPF pulses on SNM.

$k_{\text{eff}}=0.947$ best matches the data, which agrees well with expected static object MCNP-calculated value of 0.950 ± 0.004

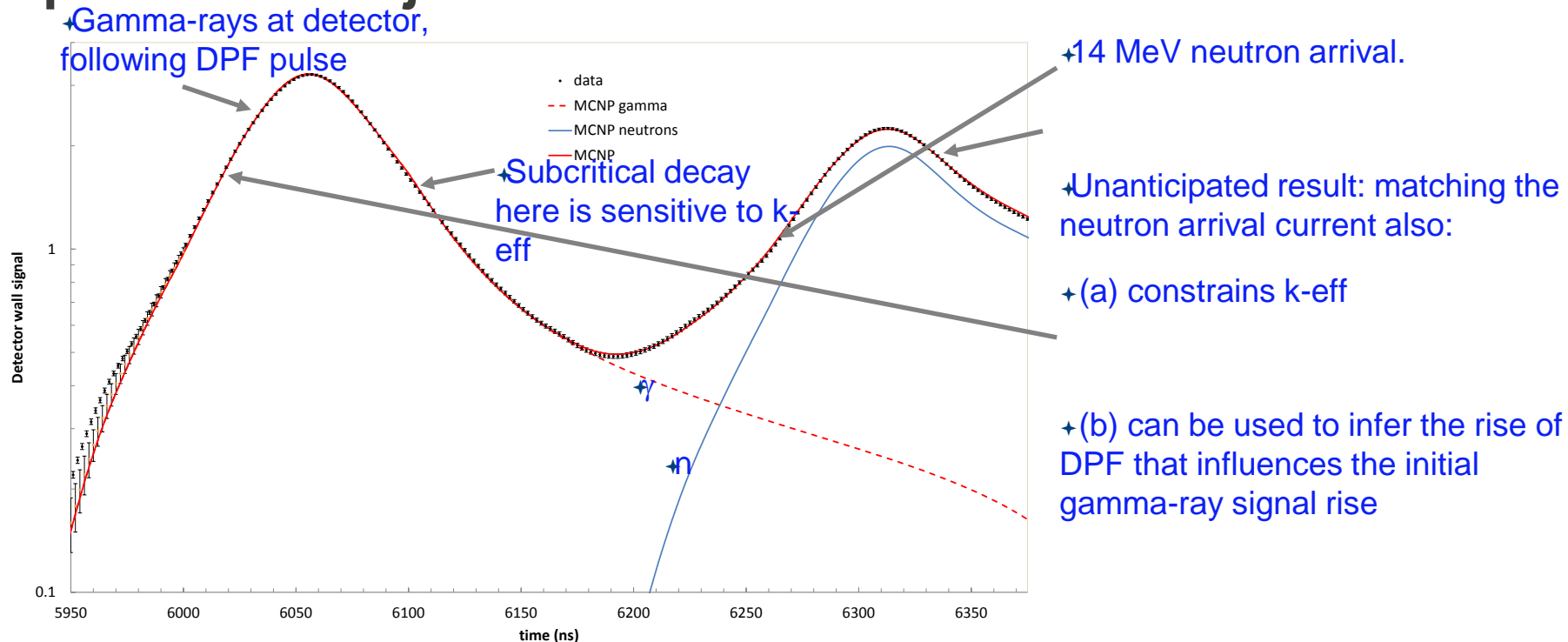


Modeling assumptions made, which require further work:

- Time constants for γ , n detection response-times
- Detector efficiency for neutron measurement
- Best way to understand DPF pulse shape, for forward modeling (close in detectors and/or scattered neutron signal)

MCNP Simulations of detectors, following 13 DPF pulses.

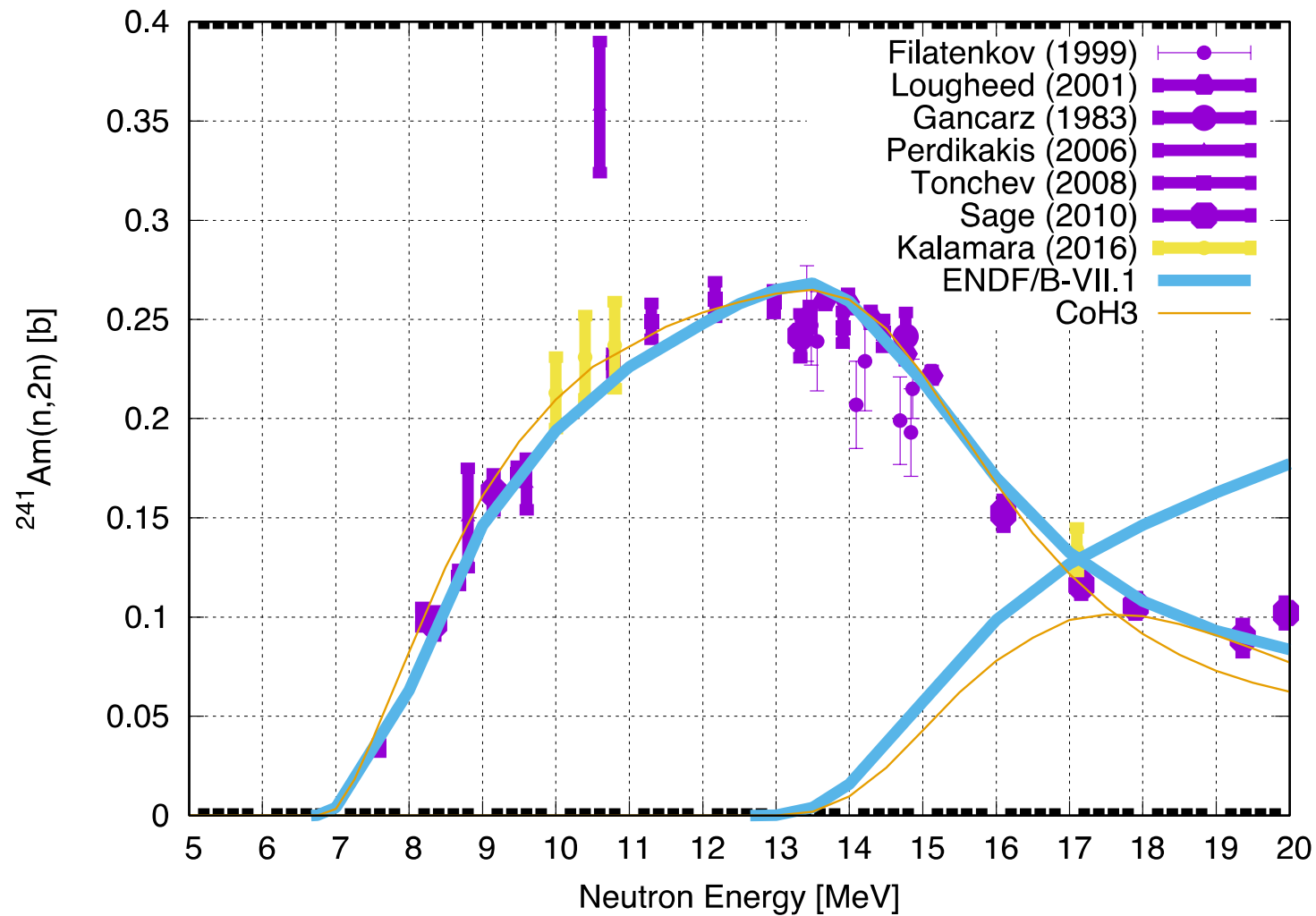
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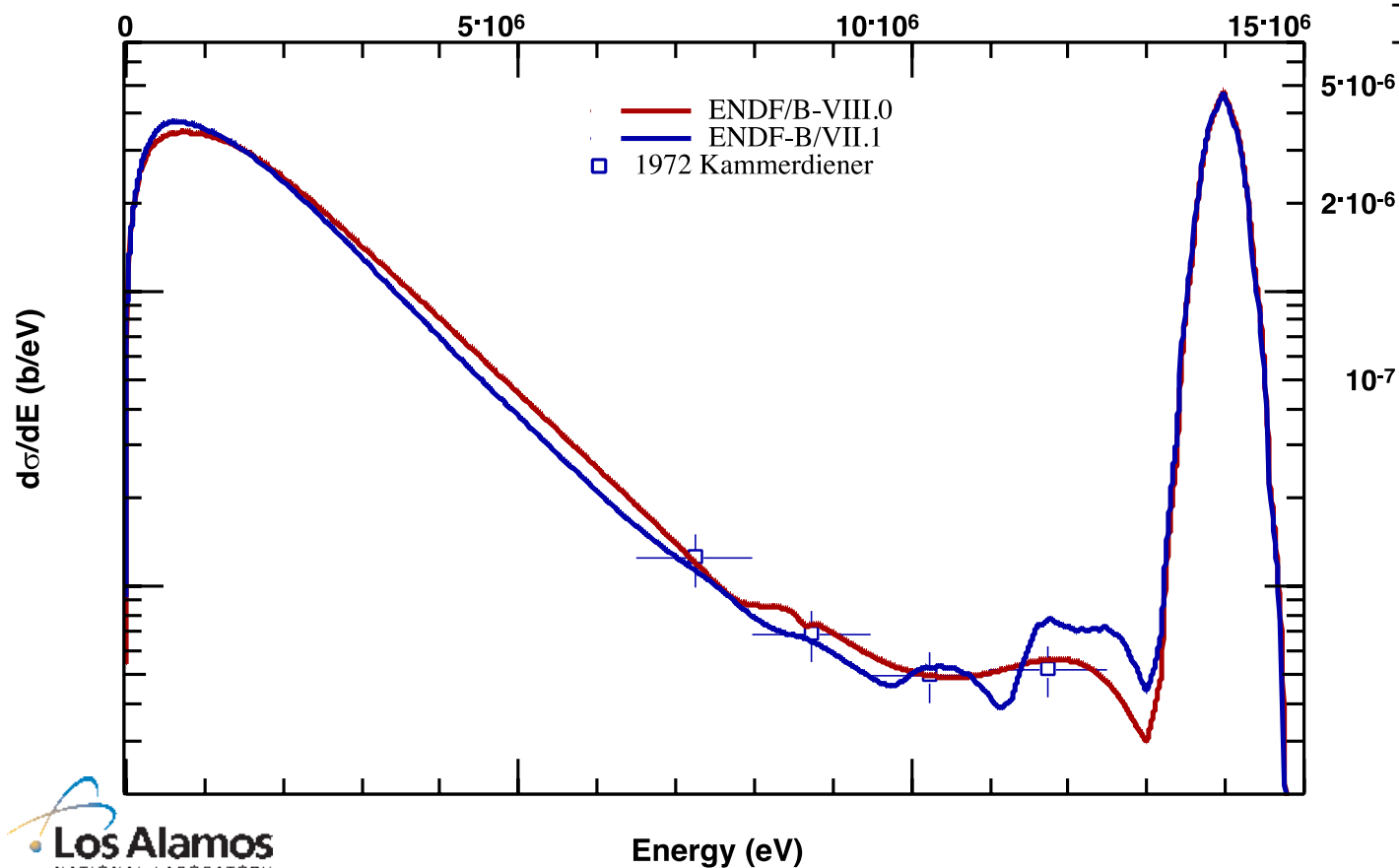
- Time constants for g, n detection response-times
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$^{241}\text{Am}(n,2n)$



235U 14 MeV scattering

92-U-235(n,x) Ei1.40E+7



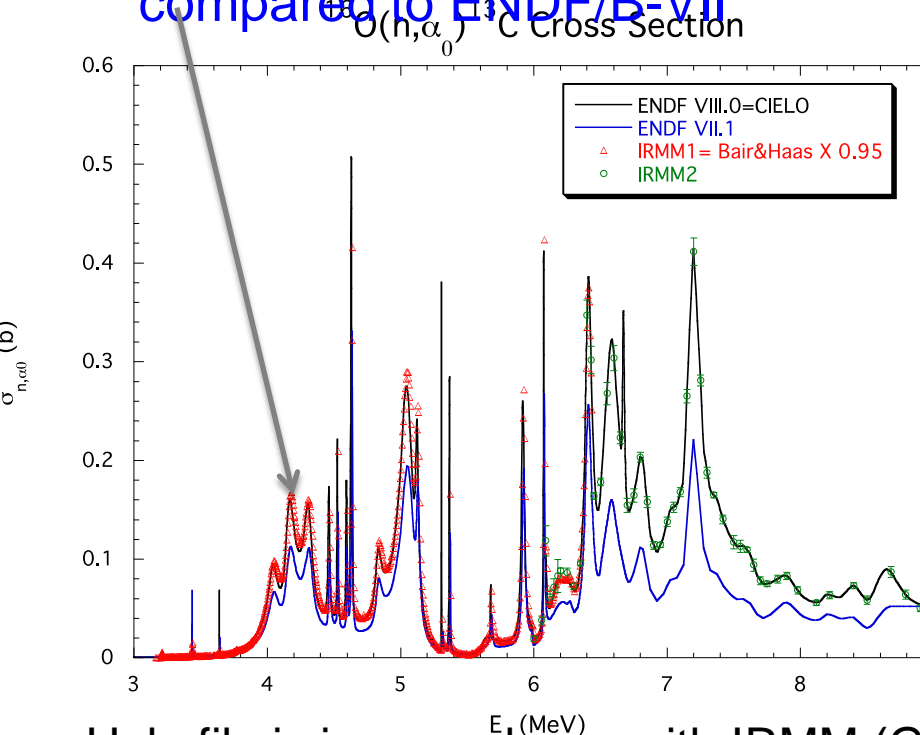
Total Inelastic at 14 MeV:

- 514 mb in VII.1
- 339 mb in VIII.0

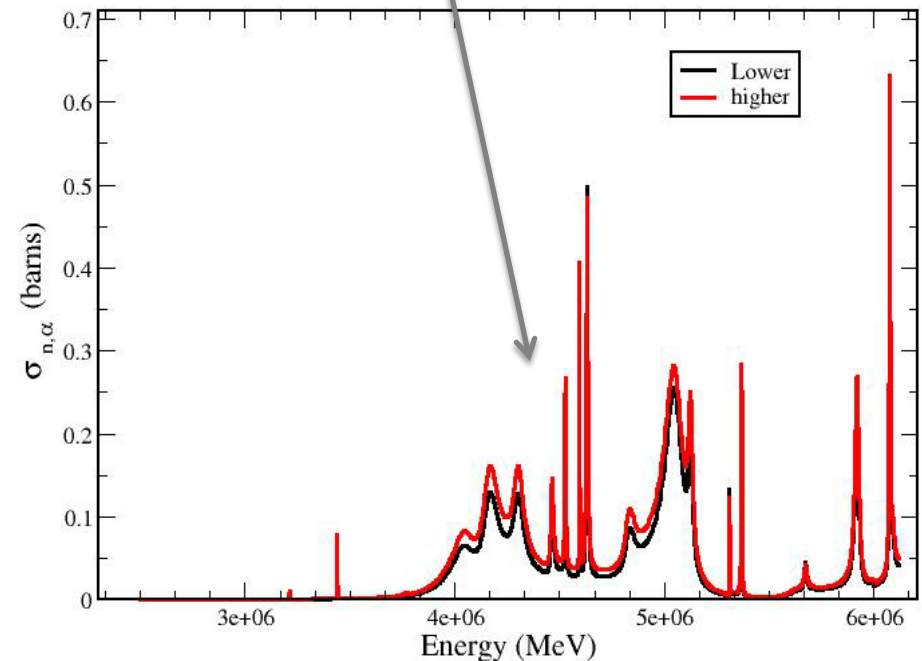
Examples of convergence of opinion in CIELO

(1) Oxygen-16 (n,α) increases, neutron absorption leading to reduced criticality

Hale increases (n,α) by ~40% compared to ENDF/B-VII



Leal “high and low” options, high similar to Hale



Hale file is in accordance with IRMM (Giorginis et al.) & Kunieda conclusions; But note, differing opinion from Marco Pigni/ORNL, who argues for lower (n,α)

Future “confirmatory” experiments started, including Los Alamos & by astrophysicists

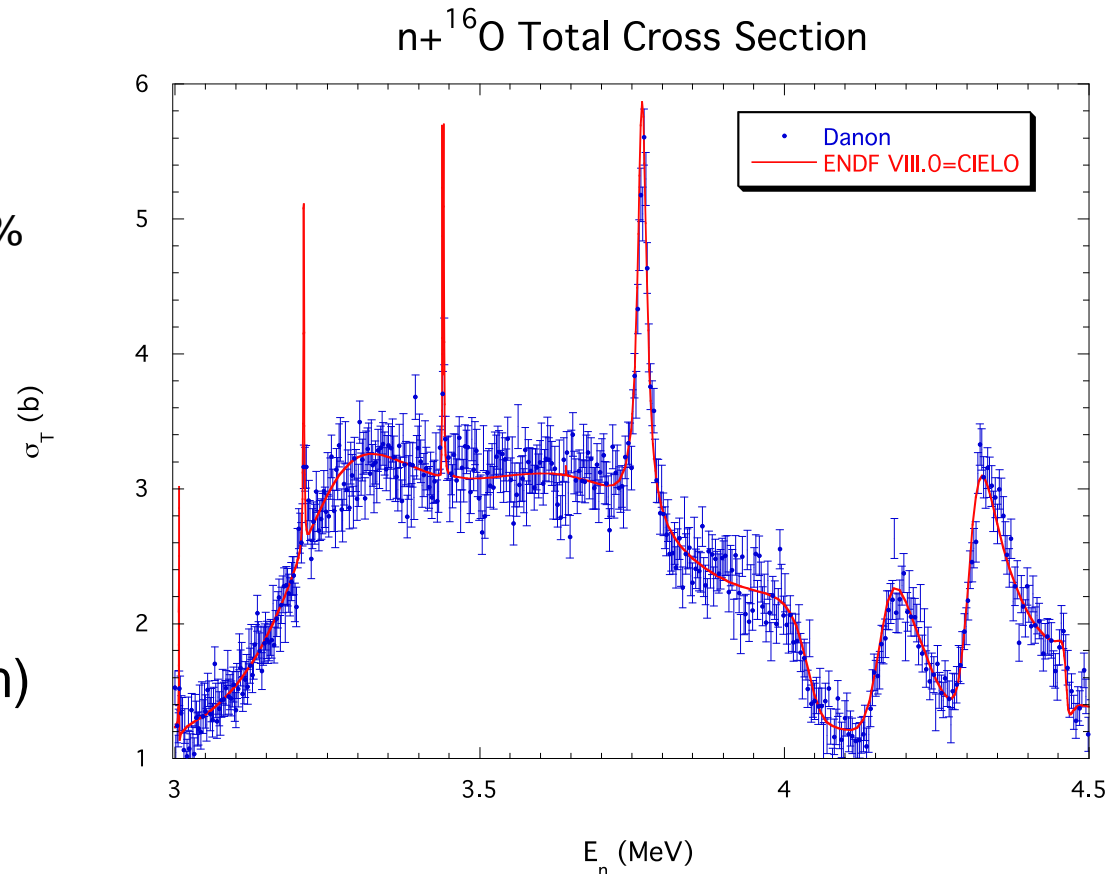
Blind test of R-matrix analysis predictive capability

Oxygen-16 total cross section, normalization determined from RPI experiment

RPI (Danon) measurement made after evaluation

- EDA code prediction agrees to <1% from 0.2-9 MeV
- *Remarkable!*

Resolves previous 3-4 % normalization uncertainties (Cierjacks'68 had correct norm)



Examples of convergence in CIELO

Oxygen-16 low-energy elastic scattering

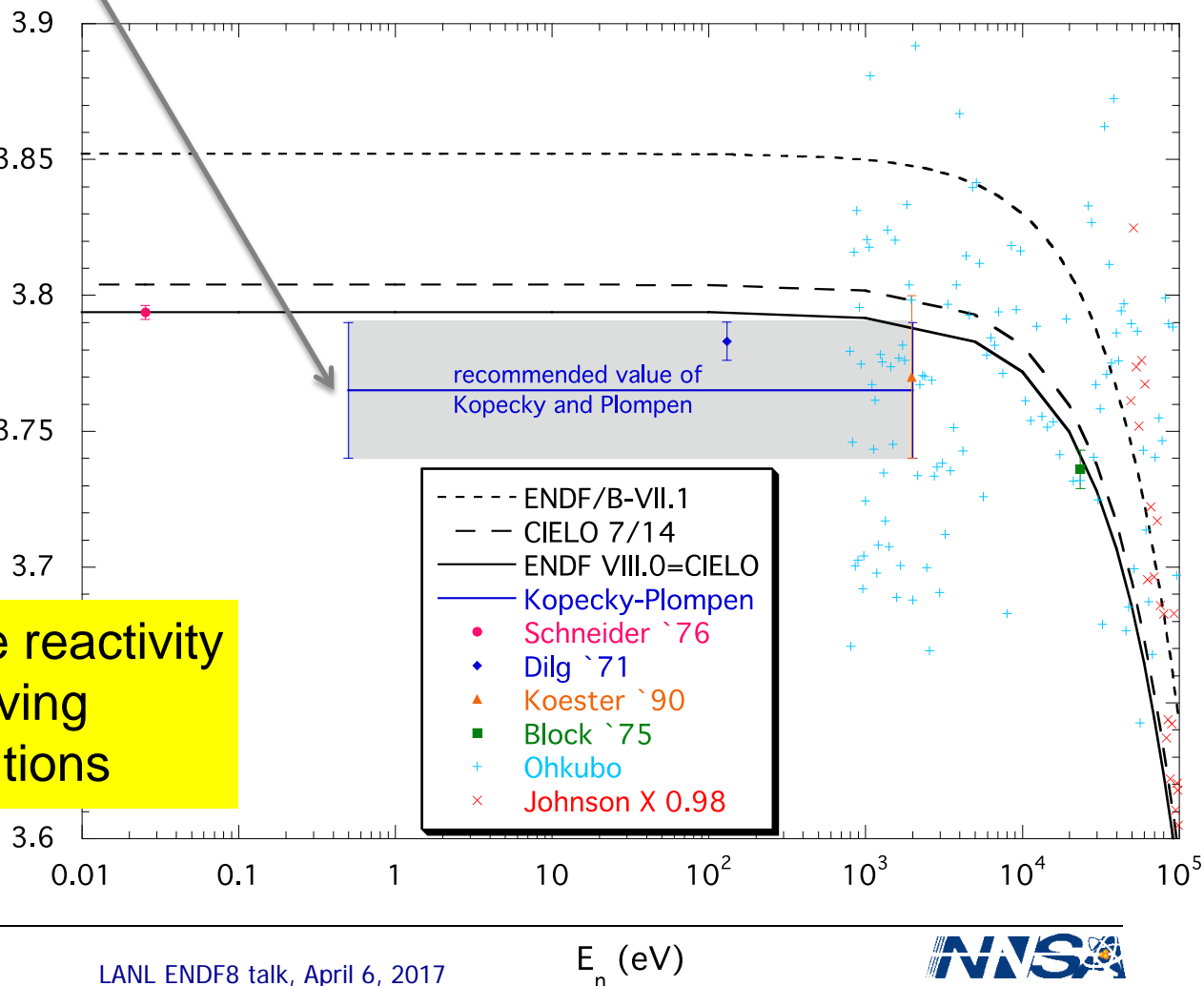
Leal adopts 3.765b at 0K

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

Hale's evaluation is somewhat higher, but still ~ 1.5% lower than ENDF/B-VII.1

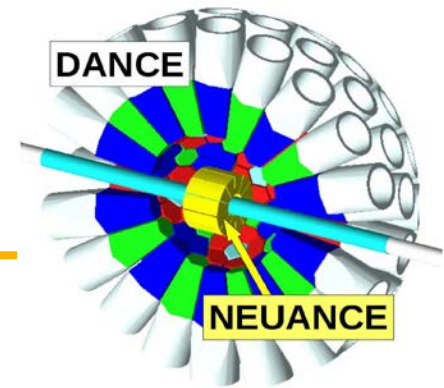
Chalk River heavy-water reactor insights useful too.

$\sigma_{el} \text{ (b)}$



These changes reduce the reactivity of critical assemblies involving oxygen – e.g. thermal solutions

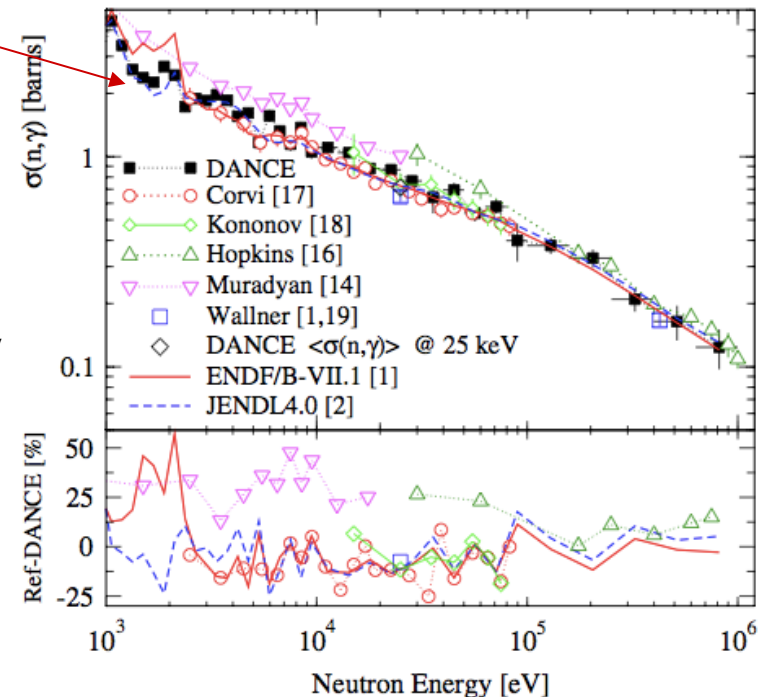
Uranium-235



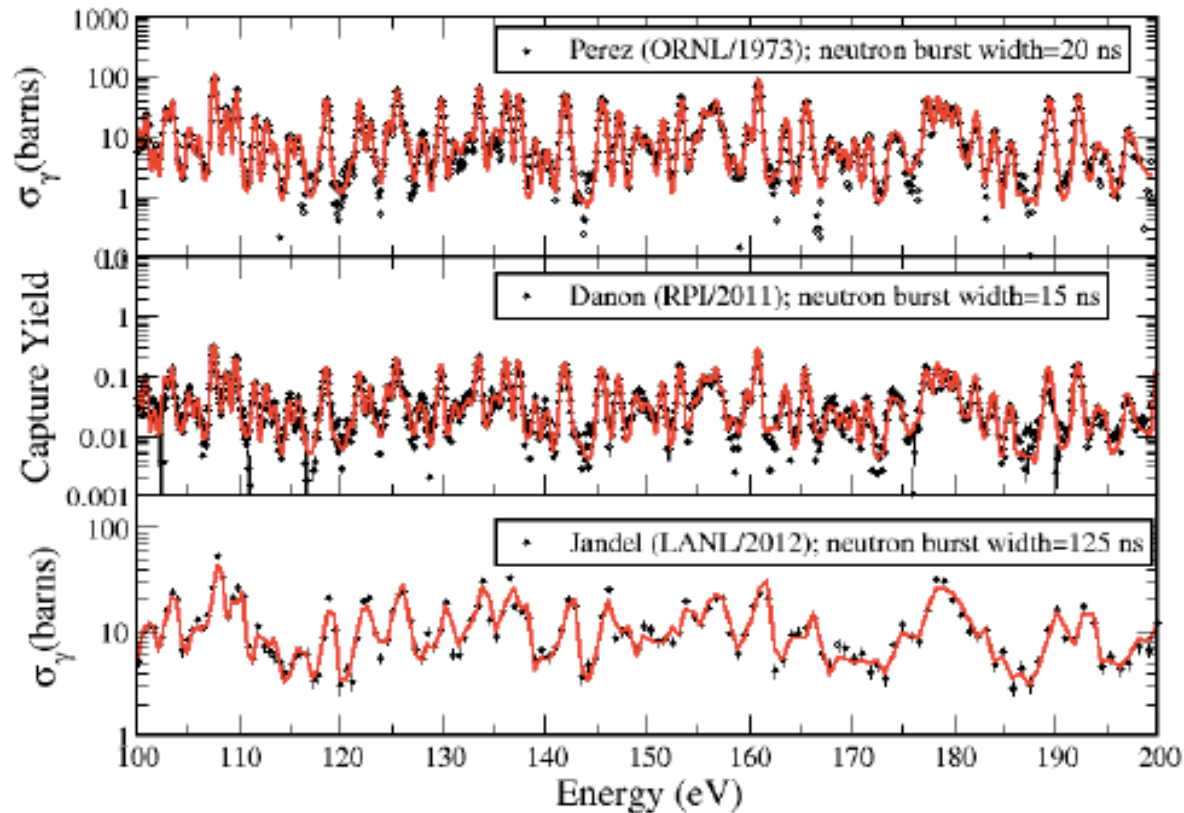
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SAMMY resonance analysis by ORNL & IRSN



Paper @ ND2016



Figure 5 : SAMMY fitting of the fission cross section in the 100 eV to 400 eV energy range.

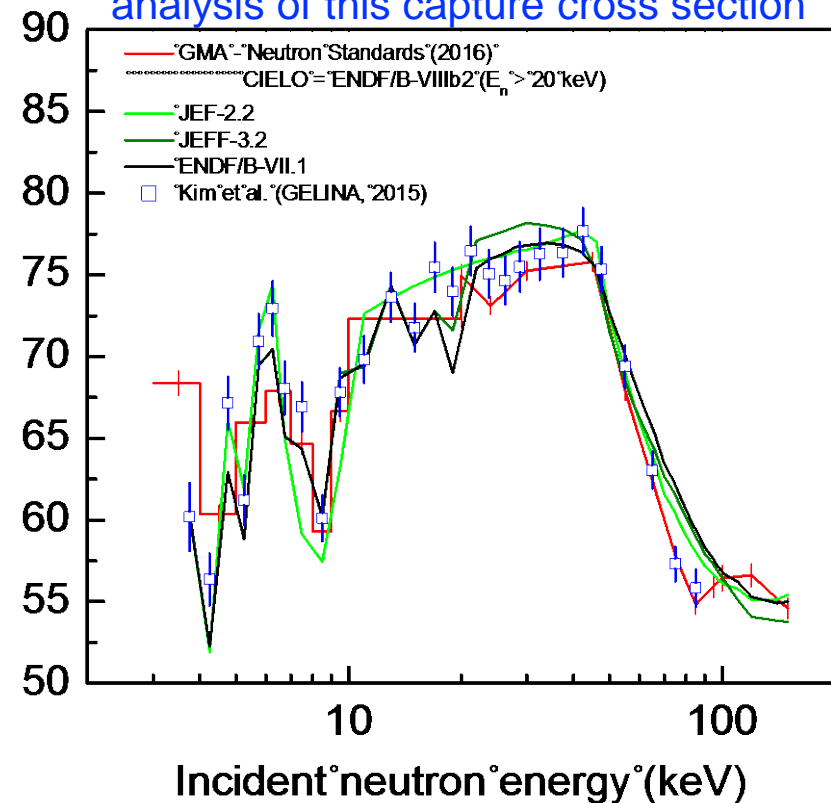
Uranium-238

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$[\sigma \times E^{1/2}]^{oo} (b \cdot eV^{1/2})$

CIELO-1 uses the new standards analysis of this capture cross section

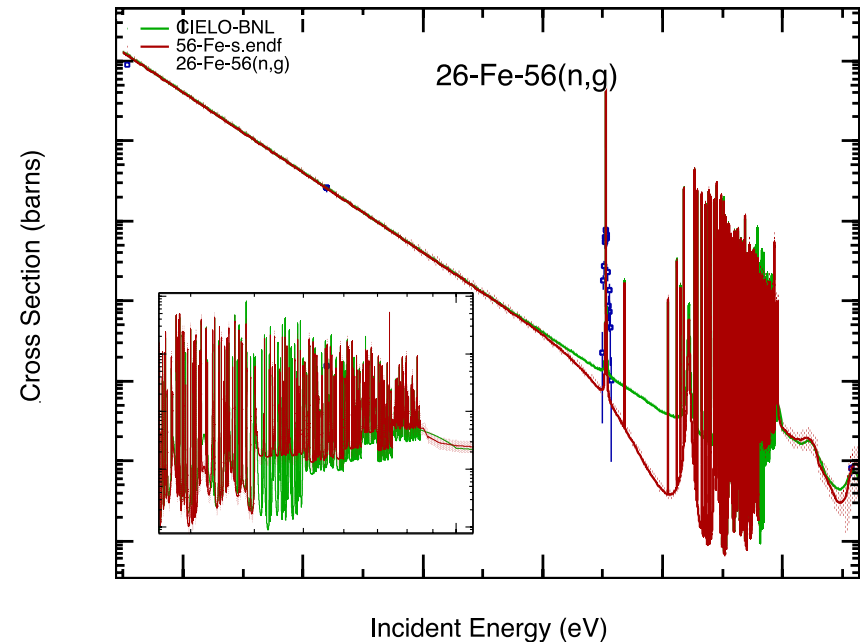


Iron-56

Challenge: careful treatment of fluctuations & angular distributions:

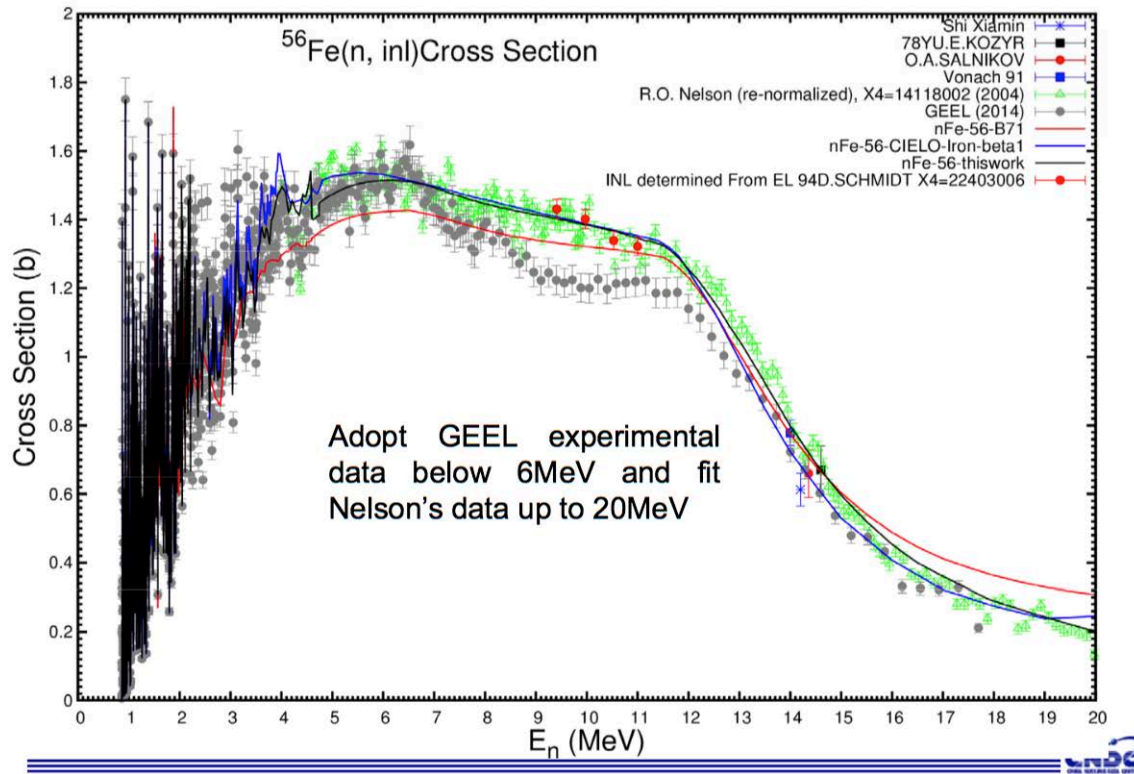
- New resonance analysis from Leal (IRNS), but just up to 850 keV in CIELO-1, and some modifications for capture.
- Followed fluctuations in Geel & other data
- Updated inelastic, and complete new statistical-model & coupled-channels analysis
- “Semi-integral RPI data”, for scattering, and RPI capture data
- New higher energy fast analysis by BNL, CIAE & JAEA

CIELO-1 radiative capture

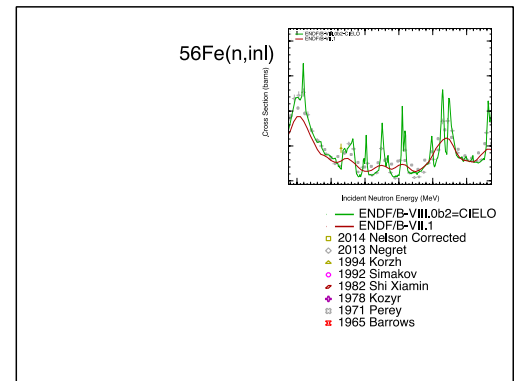


Fe-56 – Chinese evaluation of iron

Presentation for the CIELO Meeting of the NEA
9-11 May 2016 Paris, France



Increased inelastic cross section in BNL's CIELO-1



PFGS for ENDF/B-VIII

Removes 1.09 MeV discontinuity in representations. Now:

- all production gamma processes represented explicitly to 30 MeV (benefiting from IAEA Empire (U) and LANL CoH (Pu) calculational capabilities)
- Fission gammas explicitly represented for all incident energies
- Additional benefit of not having a double-counting error in MCNP simulations when fission event-generator is used!

Uses PFGS spectrum assessed at thermal, and carries over to high energies

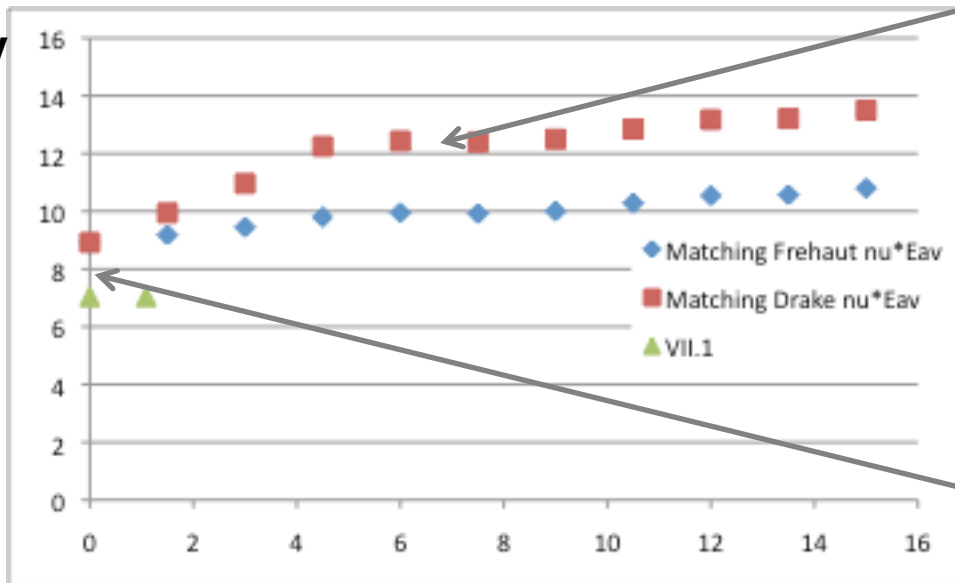
- benefits from recent data taken at Geel and LANL (235U and Pu) and 238U from France
- informed by CFGM model simulations too

Notable issues to consider, though:

- large VII.0 low-energy (<200 keV) spectrum (from calcs) results in much higher multiplicities. [extra gammas at very low energies]. Defensible?
- our study has revealed discrepancies between Drake LANL data (that informed ENDF g-production transport) & Frehaut/Fort data (used in ENDF VII.0 MT 450)

Example of PFGS issue, ^{235}U gamma multiplicity

Multiplicity



Neutron energy

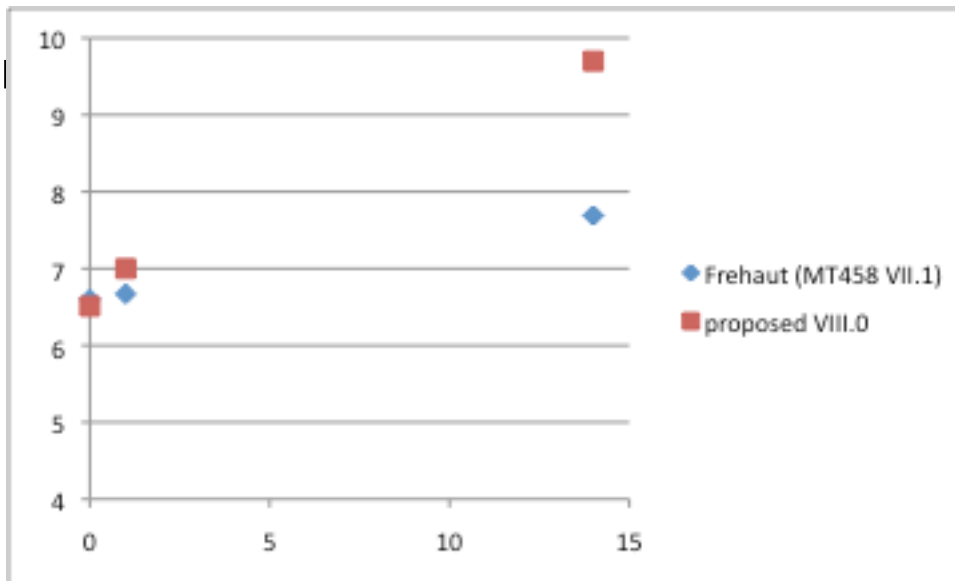
Higher - we are intentionally matching Drake, not Frehaut.

Drake LANL exp. looks good, and was previous matched in ENDF/B-VII.1 transport file.

Higher because gamma-ray diagnostics spectrum now has more photons below 200 keV, so fewer above 200 keV, implying need for higher nubar, to still match data >200 keV

Example of PFGS issue, ^{235}U gamma energy per fission

Energy
Per-fission
MeV



Neutron energy

✦ Even though proposed VIII.0 is much higher @ 14 MeV than Frehaut ,

✦ ENDF/B-VII transport file actually was similar to the proposed red points (though did not represent fission explicitly above 1.09).

✦ In VIII.0, we can now make the photon production and MT458 consistent.

✦ Implication will be to