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CSEWG 2012: Evaluation Plans for ENDF Updates

M.B. Chadwick

X-CP Computational Physics Division, LANL

Overview

International ENDF files? (CIELO project)

Priorities for next version of ENDF/B

- my suggestion is focus on small number of high impact isotopes

- making cross section updates whilst preserving/improving criticality performance will be a major challenge

- also address deficiencies identified by data testers (CSEWG, VDM paper, SG33 *etc*), especially “low hanging fruit”

Examples of issues to address, & time lines

Present funding agency priorities at LANL (National Security, Crit Safety, DOE/Science

-Criticality, fission, capture, UQ/QMU, diagnostics, Standards, TN, GS needs

-- Gaps/Smaller focus: reactors, (Ex states, HEDP nuc science – LLNL)

Acknowledgment: Contributions from Kawano, Jandel, Talou, Herman, Pritychenko, Go Chiba, Nagaya, ….

CIELO: Collaborative International Evaluated Library Organization – Presented to IAEA & WPEC in 2012. Pilot Project Started – We'll be meeting at the NEA in Nov

- **Nuclear data are physical constants – there's only one correct answer!**
  - Existing ENDF, JENDL, JEFF, …. have reached a level of maturity to enable us to contemplate this next step – *they're already converging!*
- **Quality: new advances will benefit from being a collaborative product from the world's best experts – pool our resources**
- **Computational/methods advances enable a "step function" in improvement, exploring the large phase space of solutions using UQ and covariance methods**
- **We have mid-career experts to shepherd this project through, and some key retirees who may be able to help**
- **Build on initial steps already taken through international collaborations**
  - IAEA/WPEC standards; RIPL; Dosimetry; Photonuclear; U8 capture; FPs; CEA-ORNL resonances…

Pilot Project – Is CIELO Feasible? Can the Community Make this Work? Do they Value it?

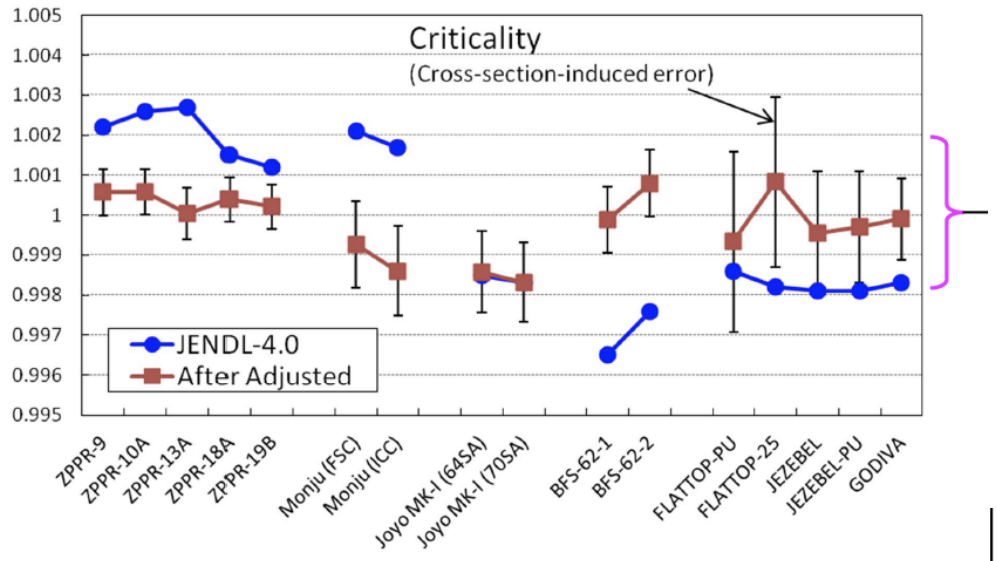
- ✓ **Initial Pilot Project Focus on 1H, 16O, 56Fe ^{235,8}U and ^{239}Pu, with a goal to make substantive advances within 2-3 years**
- ✓ **Identify discrepancies – there are many complex issues to address**
- **Establish teams of ENDF, JEFF, JENDL, IAEA, … specialists to work on each nucleus**
- **Resolve discrepancies and create new CIELO files: Insights come from experiment (cross sections, spectra, integral experiments), theory, simulation**
- **Maintain good integral validation performance (k-eff criticality, reaction rates, etc) while having more physically-justifiable cross section representation**
- **Based on initial experience, consider expanding the CIELO concept – more nuclei, more people involved, formal plans, etc**

LANL Priorities for ENDF/B – 4-5 Years Away. These are Probably Common Priorities for all Countries

- **Refine covariances**
- **Big 3: ^{235,8}U and ^{239}Pu:** Remove compensating errors likely present in current ENDF, JEFF, ENDL evaluations (between fission, PFNS, elastic, inelastic, capture, nubar, resonance, … reactions), and improve key reaction channels (PFNS, fission, capture, inelastic & elastic)
- **^{16}O, ^{12,nat}C, (^{23}Na, ^{56}Fe, ^{90}Zr – esp. BNL)**
- **Expand ENDF data for nonproliferation/SNM detection applications**
- **Exploit measurements – those made in the next 2-3 years**
- **Address whether feedback from Adjustment/Covariance efforts point to any cross section changes (SG33, Commara, Japanese ADJ file, etc)**
- **Ensure consistency with IAEA dosimetry data; New Standards**
- **Validation feedback on issues:** Pu-solutions & intermediate energies; Fast Be, Ni, V reflectors; Thermal Pb reflectors. Fast Pb too; (VDM-Fe, Cd, Gd though we have tried here for VV.1)
- **? Continue improvements of MA; neutron+ FPs, & FPYs, KERMA**

Japan & USA data adjustment – are there any lessons for us regarding the underlying cross sections?

Cross-Section Adjustment (3/3)
Performance of ADJ2010



Predict the criticality of various cores within 0.2%dk.

Evaluation and Improvement of Design Accuracy of FR Cores

Accuracy of a Large FR Core Design
(Contribution from cross-section error before (B) and after (A) adjustment)

A 750 MWe-class sodium-cooled MOX core (diameter: ~3.5m, height: 1.0m)

Error and Components	Criticality		Burnup Reactivity	
	B	A	B	A
Total Error	0.87	0.19	5.7	3.6
Pu-239 fission spectrum	0.40	0.19	1.0	0.5
Fe Inelastic	0.30	0.13	0.9	0.4
U-238 Capture	0.34	0.15	3.6	1.6
U-238 Inelastic	0.40	0.13	0.7	0.5
Pu-239 Capture	0.18	0.12	1.8	1.2
Pu-239 Fission	0.25	0.17	0.4	0.3
FPs of Pu-239 Capture	0.12	0.12	2.1	2.1
Beta of U-238	-	-	1.4	1.0
Beta of Pu-239	-	-	1.0	0.9
Others	0.35	-0.33	3.2	2.0

unit: % (1 sigma)

Total errors are remarkably reduced by adjustment

The contribution of each isotope is also clarified.

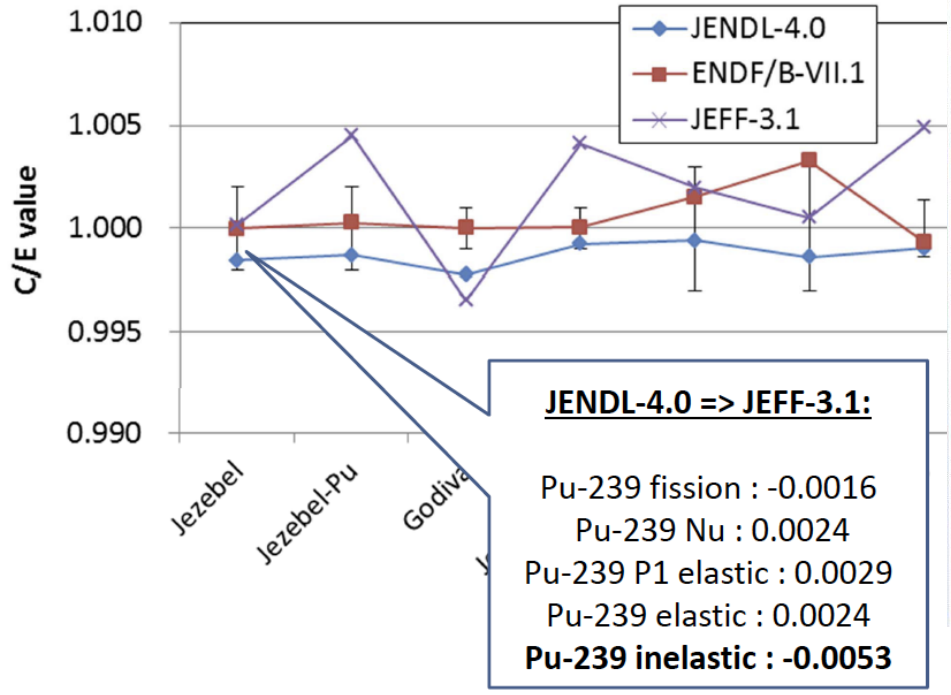
Note, these are all reactions we aim to improve for CIELO and for the next ENDF!

(Consistent with conclusions from INL Commara2 adjustment, where the biggest issues for future work were: U5 capture, u8 pu9 inelastic, 237Np fission and FP captures)

Differences in Reasons for Fast Plutonium Criticality

Japanese analysis

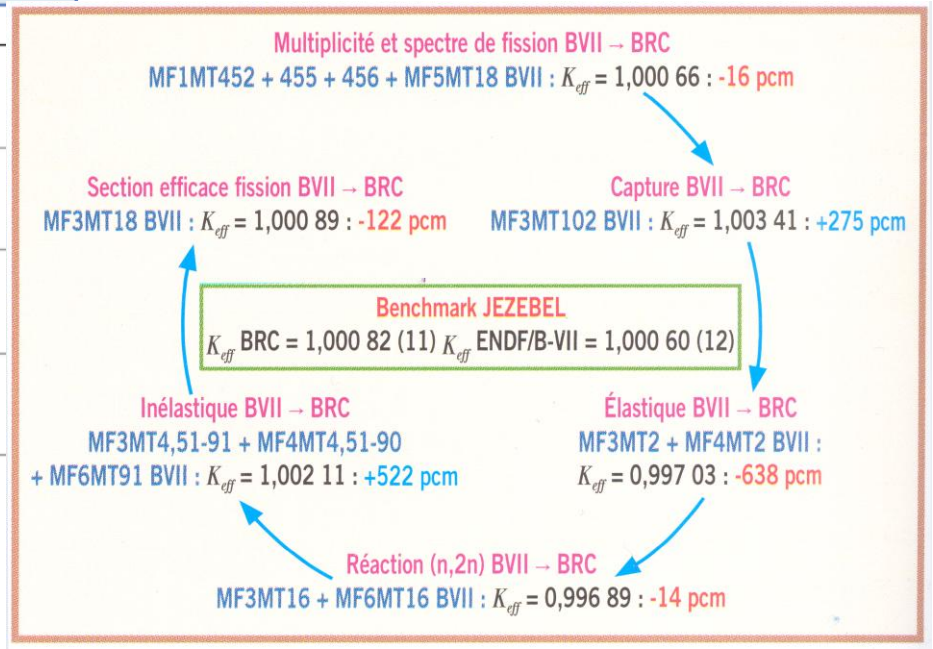
Very small fast systems: Now



JENDL-4.0 => JEFF-3.1:

Pu-239 fission : -0.0016
Pu-239 Nu : 0.0024
Pu-239 P1 elastic : 0.0029
Pu-239 elastic : 0.0024
Pu-239 inelastic : -0.0053

CEA analysis



Inelastic & elastic are modeled very differently. (PFNS effect would be larger except all evals use a similar approach)

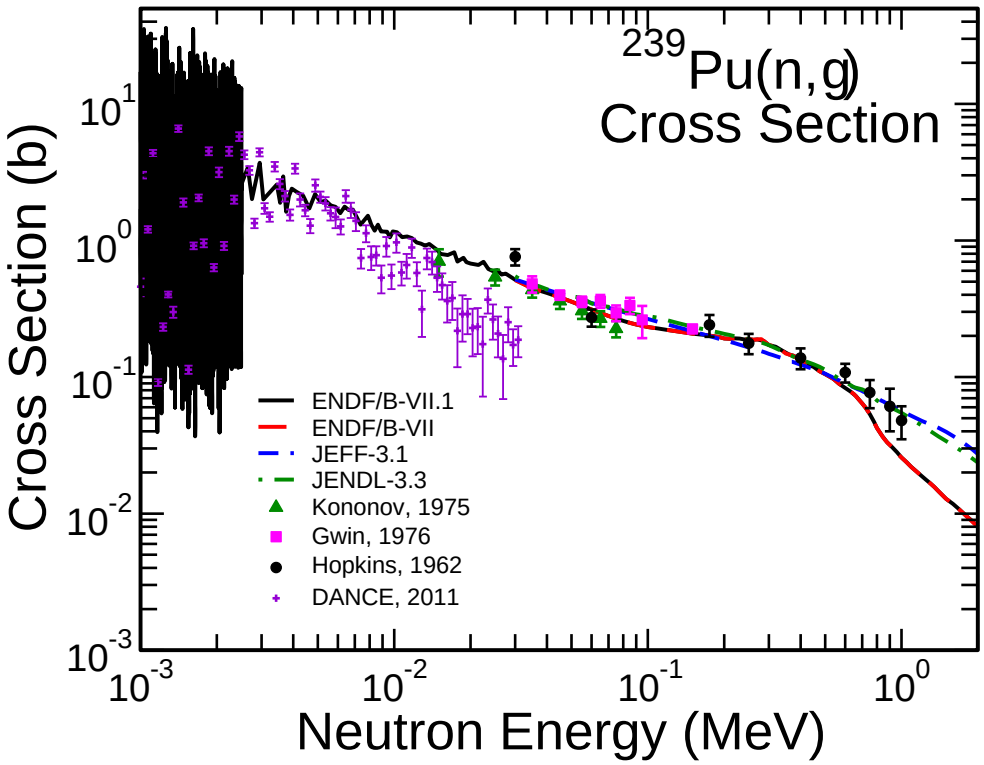
Lessons Learned Regarding How Integral Experiments Can Guide Understanding of Fundamental Cross Sections

- **Measurements that focus on just one reaction channel provide important feedback/guidance**
  - Fission rates, capture rates, n2n rates in critical assemblies, well-defined sources (e.g. Cf, 235U-thermal, …), and sometimes in reactor experiments
  - Hard to disentangle spectrum effects on threshold fission rates (e.g. inelastic v. PFNS)
- **K-eff criticality analysis of experiments tends to have too many inverse solutions (under-determined) to determine cross section**
  - Thus, most adjustment projects do not provide consistently-reliable feedback on cross sections (exceptions? – 235Un,g near 1 keV from Japan; 238U resonances ?)
  - But perhaps with broader suites of differing types of experiments, with increased computational UQ/sensitivity studies, some progress can be made
- **LANL is exploring whether subcritical neutron multiplication experiments provide focused feedback on nubar, or whether they are "more like k-eff"**
- **In sensitivity studies for k-eff, "everything matters"!**
  - Angular distributions (> than just P1), PFNS, energy spectra all matter, as well as x/s
  - "The adjustment process works on just what it has" (McKnight)

^{239}Pu. Much Work is Needed, As We Seek To Maintain Good Fast Criticality Performance and Improve Intermediate (ZPR) and Thermal Performance

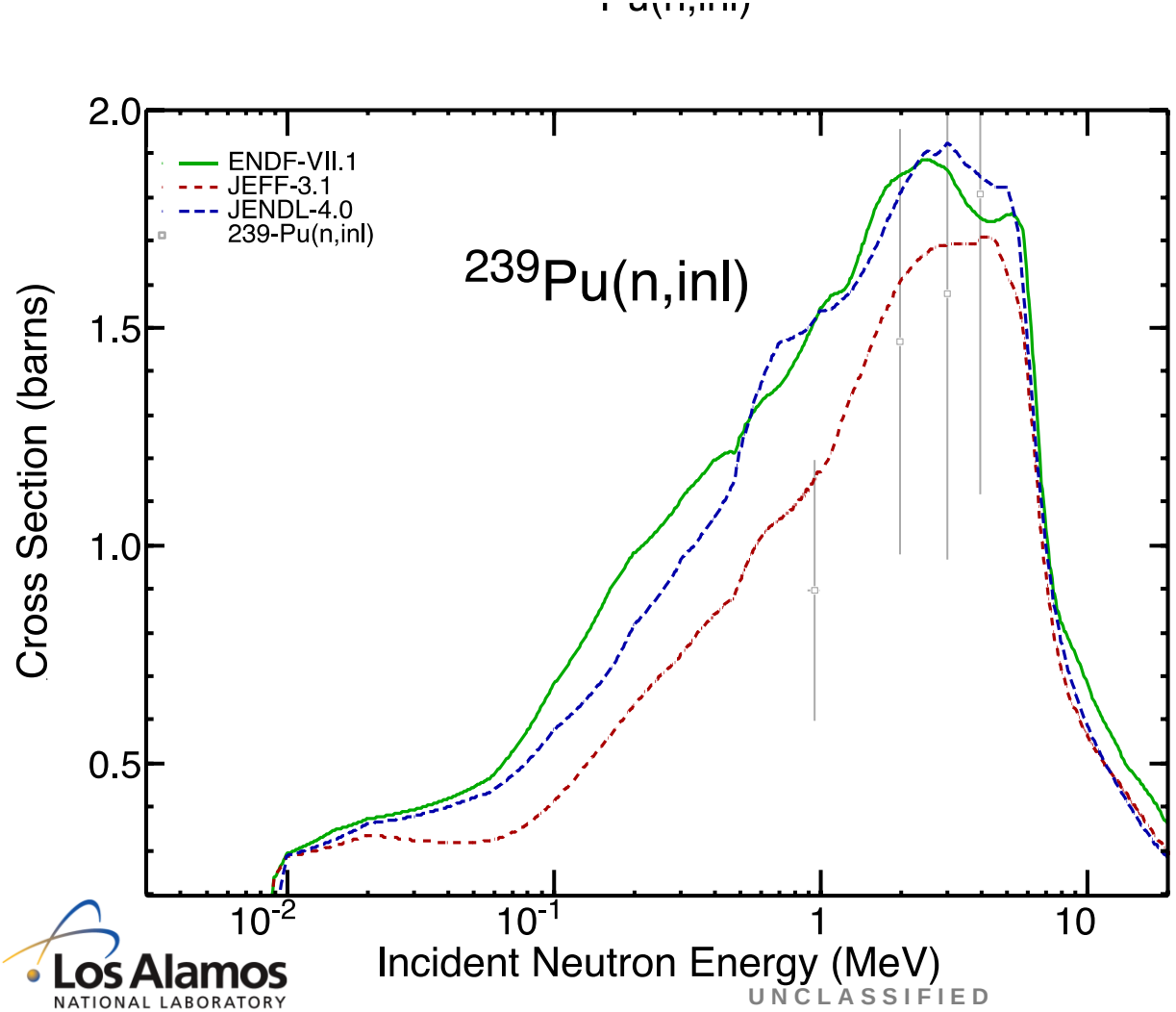
	Reaction channel		Issues
✓	Capture	2012,13	10%+ discrepancies in the 1kev – MeVs region. Few data exist and they are discrepant; New DANCE data may be available in 1-2 years. PROFIL suggests ENDF/B-VII.1 capture is overall ~ 10% low.
✓	Inelastic, xs; ang dist	2012,13	Large differences with JEFF in the kev – MeV region, with less measured data than we would like. Theory/modeling advances will likely contribute importantly
	Elastic, xs; ang dist	2012,13	Large differences with JEFF
	(n,2n)	2012,13	ENDF and JENDL similar and agree with the GEANIE measurement, JEFF different. PROFIL suggests a significant change near threshold, but LANL disagrees
	Fission – cross section	2012-17	Significant differences, outside the Standards assessed uncertainties. TPC data will be available in 5+ years!
	Fission – nubar	2012,13	ENDF should remove the tweak we made to match Jezebel (a small increase in the fast region). Subrit multiplication experiments support removing this. Consider if thermal changes are warranted (Koning/Rochman search gave a 3-sigma lower value)
	Fission – PFNS	2013-14	LANSCE data (LANL, LLNL, CEA), with theory, dosimetry, and nuex data, and with IAEA CRP, will determine the PFNS more accurately by ~ 2014
✓	PFGS for γ & multiplicity	2013	DANCE data (in 2012-2013) should be used to replace/update the existing PFGS. Also, fission gammas should be represented at all energies, not just up to 1.09 MeV
	P(nu), Chi(nu) for n,γ	2013?	Could be added for detection applications, based on measured data (incl new DANCE data for g), Lestone's routines; and on model calculations such as FREYA, CGM, …
	Resonance region	2013	ORNL/CEA updates should be adopted if possible.

Plutonium Capture: We need smaller uncertainties at 1 keV and in the fast (100-1000 keV) range



- 1 KeV needs to be better determined
- 100-1000 keV: needs to be better understood:
  - Existing uncertainties >15%
  - PROFIL (PHENIX) 238Pu(n,g) integral testing suggests B-VII is ~ 10% low over this fast reactor spectrum
  - CEA/BIII and ENDF evaluations different
  - At present, DANCE are too high. Future work may address this
  - O. Bouland (CEA) interested

Plutonium Inelastic Scattering: Large discrepancies need to be resolved

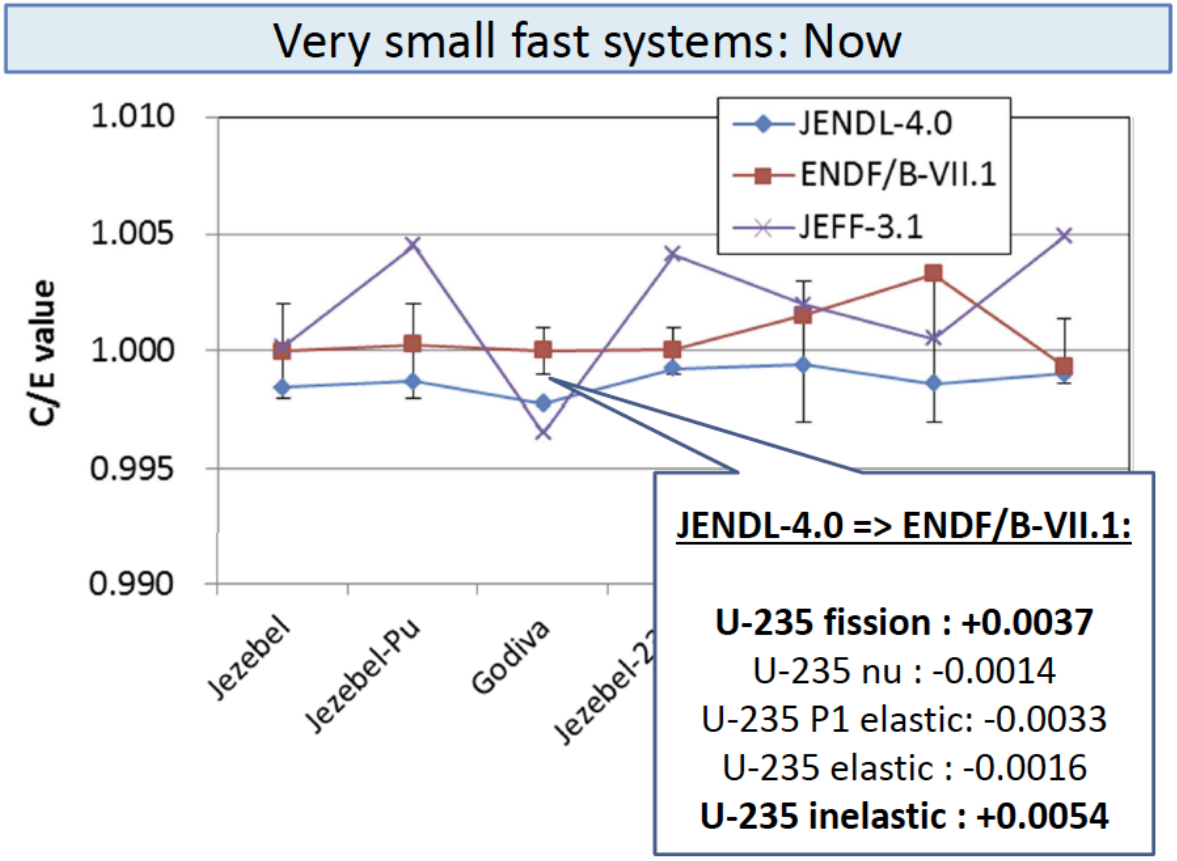


ENDF, JEFF, JENDL need to collaborate to investigate resolution of these discrepancies. Insights from CC scattering theory, KKM, *etc* will be beneficial

In the 14 MeV region, would be good to update the present pseudo-state analyses, for all the major actinides

Differences in Reasons for 235U Criticality

Japanese analysis

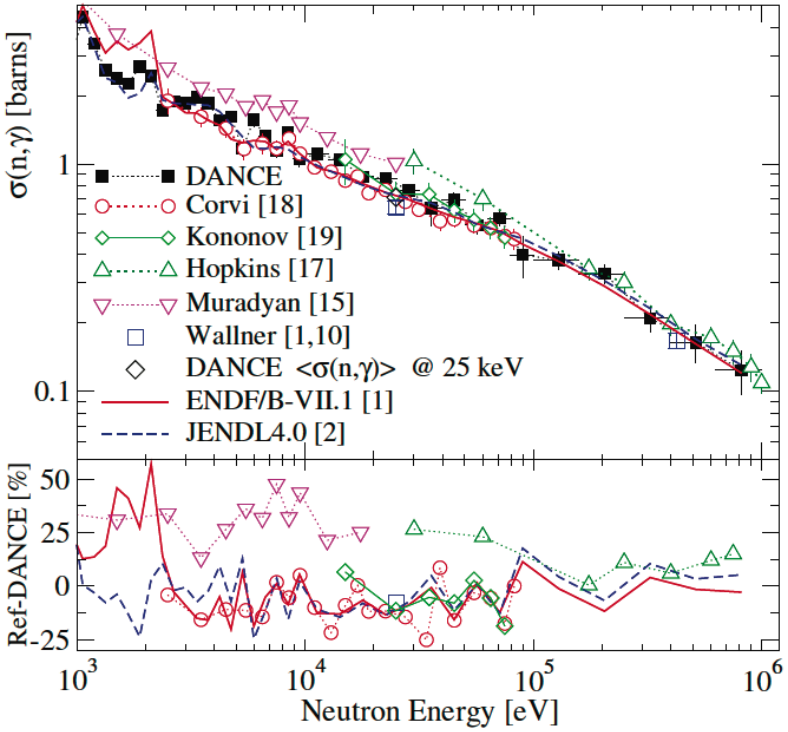


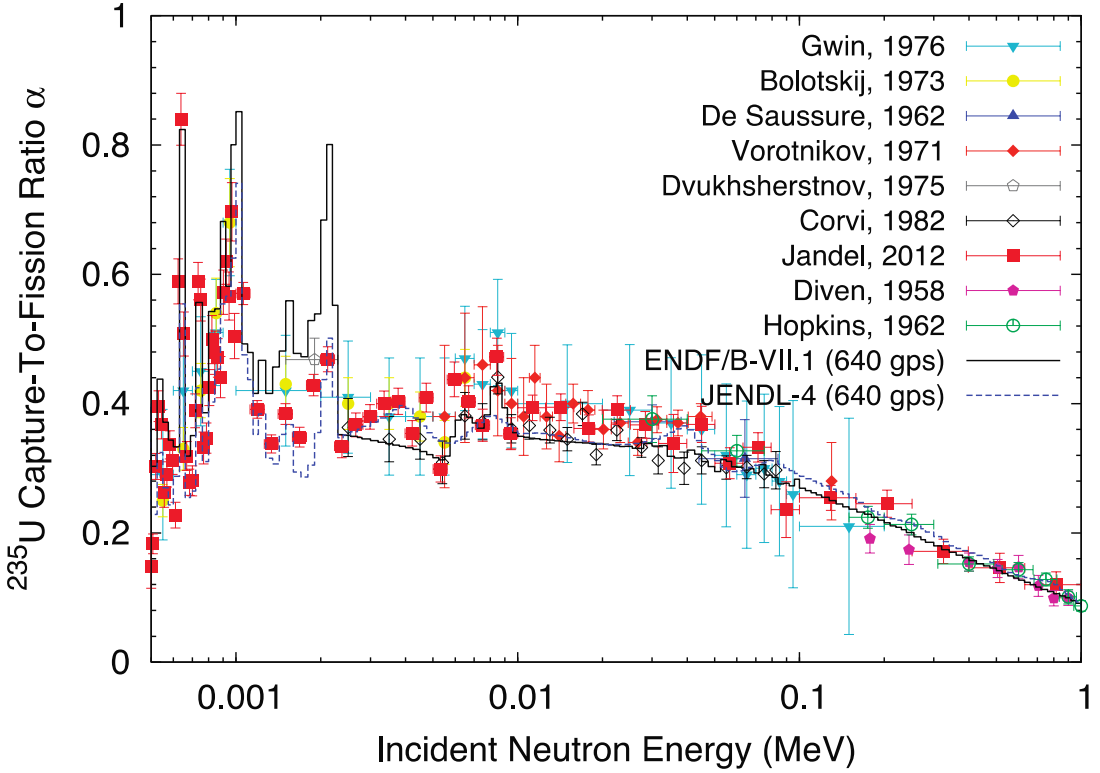
Inelastic & elastic are modeled very differently. (PFNS effect would be larger except all evals use a similar approach)

^{235}U. Much Work is Needed, As We Seek To Maintain Good Fast and Thermal Criticality Performance

	Reaction channel	Issues
✓	Capture	25%+ errors in the 1kev – MeVs region, as noted by JENDL and now corroborated by DANCE measurements. DANCE also points to ~10% level changes in the 10s - 100s keV region.
✓	Inelastic, xs and ang dist	Modest differences below a few MeV region, but bigger differences at higher energies. Discrepancies exist with the (few) measured. Theory/modeling advances will likely contribute importantly
	Elastic, xs and ang dist	TBD
	(n,2n)	Modest differences; various evaluations tend to agree with Frehaut & GEANIE data
	Fission – cross section	Significant differences, outside the Standards assessed uncertainties. TPC data will be available in 5+ years!
	Fission – nubar	Differences. ENDF should remove the tweak we made to match Godiva. Also at thermal we have tweaked nubar from the Standards value, for reactor performance.
	Fission - PFNS	LANSCE data (LANL, LLNL, CEA), with theory, dosimetry, and nuex data, and with IAEA CRP, will determine the PFNS more accurately by ~ 2014
✓	PFGS for gammas	DANCE data (in 2012-2013) should be used to replace/update the existing PFGS. Also, fission gammas should be represented at all energies, not just up to 1.09 MeV
✓	P(nu), Chi(nu) for n,g	Could be added for detection applications, based on measured data (incl new DANCE data), and on model calculations such as FREYA, CGM, …
	Resonance region	ORNL/CEA updates should be adopted if possible.

^{235}U radiative capture advances – ENDF needs upgrading in the resonance & fast regions. It appears the Japanese were right near 1 keV

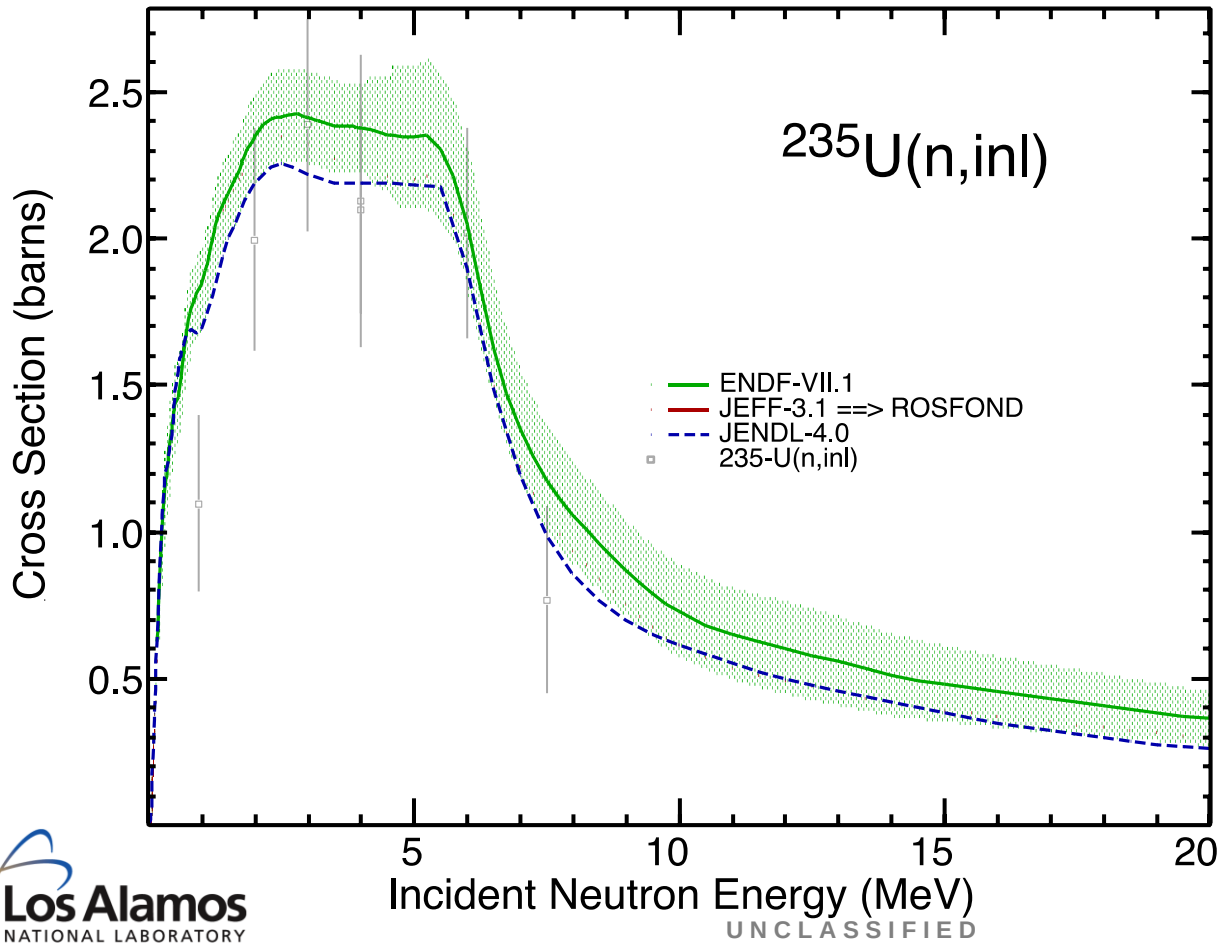




DANCE suggests ENDF too high near 1-2 keV and too low 10-40 keV

- But Wallner AMS 25 keV has ENDF high by 5% (+/- 6%); 423 keV ENDF high by 8% +/- 8%
- PROFIL fast reactor has ENDF low by 3-5%

235U Inelastic Scattering: discrepancies need to be resolved, but differences are smaller than for 239Pu

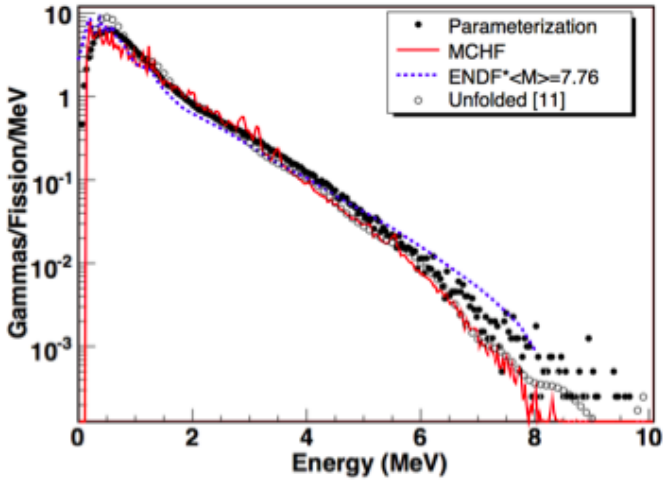


Even though differences appear small, the ENDF-JENDL difference led to 540 pcm difference in Godiva criticality!

Angular differences, and individual inelastic channel cross section differences may also play a role

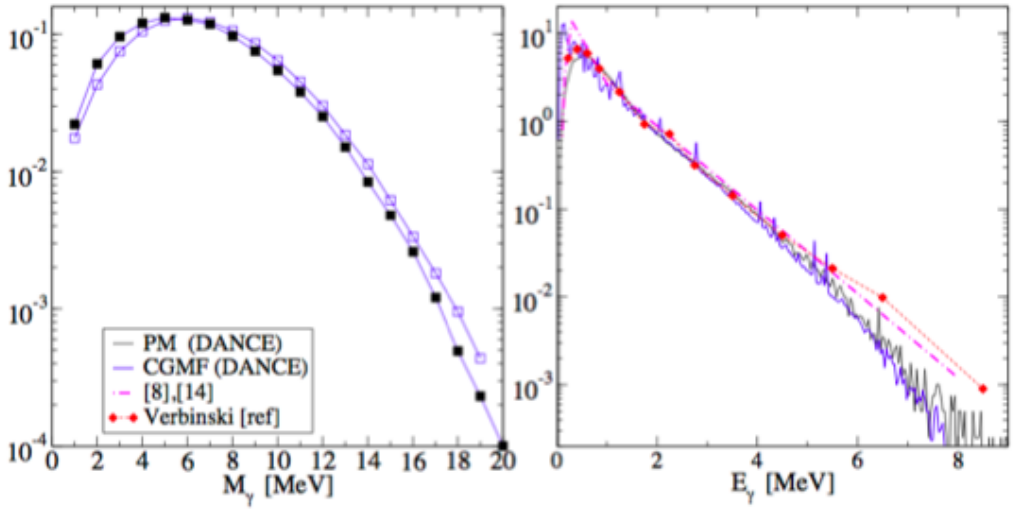
Prompt Fission Gamma Spectra from DANCE Enable an ENDF-Update. (Additionally, Multiplicity Distributions and Spectra (nu) Could be Added for Detection Applications)

^{239}Pu (n,f)



Talou calc. Multiplicity distributions are needed for SNM detection applications

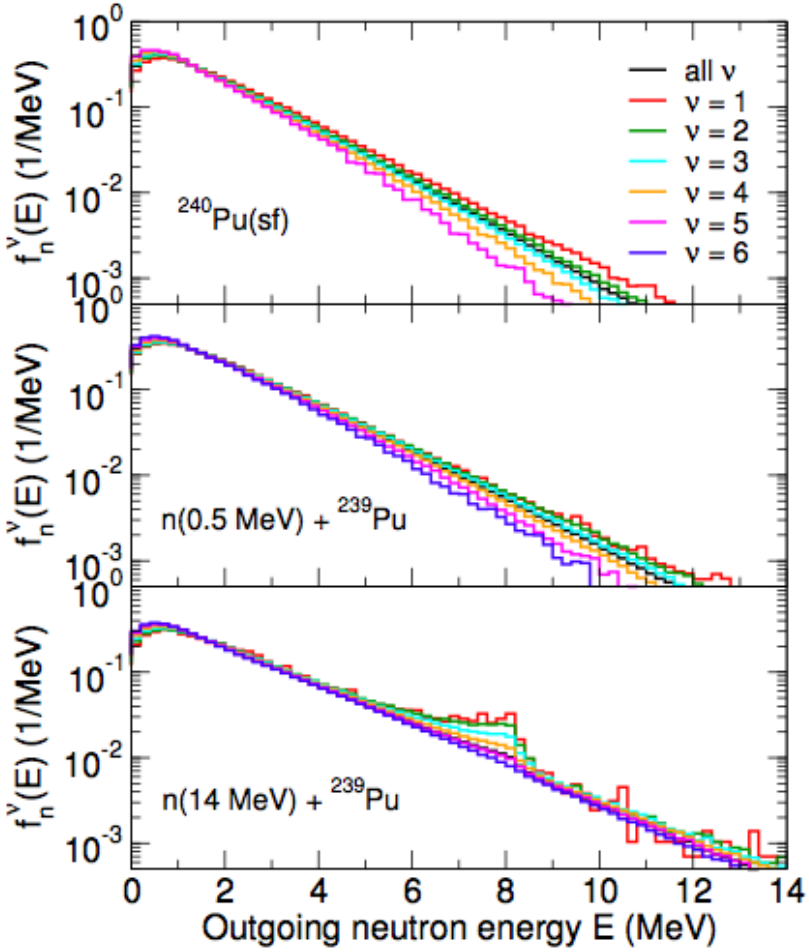
^{235}U (n,f)



J.Ullmann *et al.*,
"Prompt Gamma-Ray Production in Neutron-Induced Fission of 239Pu", to be submitted to PRC.

M.Jandel *et al.*,
"Prompt Gamma-Ray Emission in Neutron-Induced Fission of 235U," to be submitted to PRC.

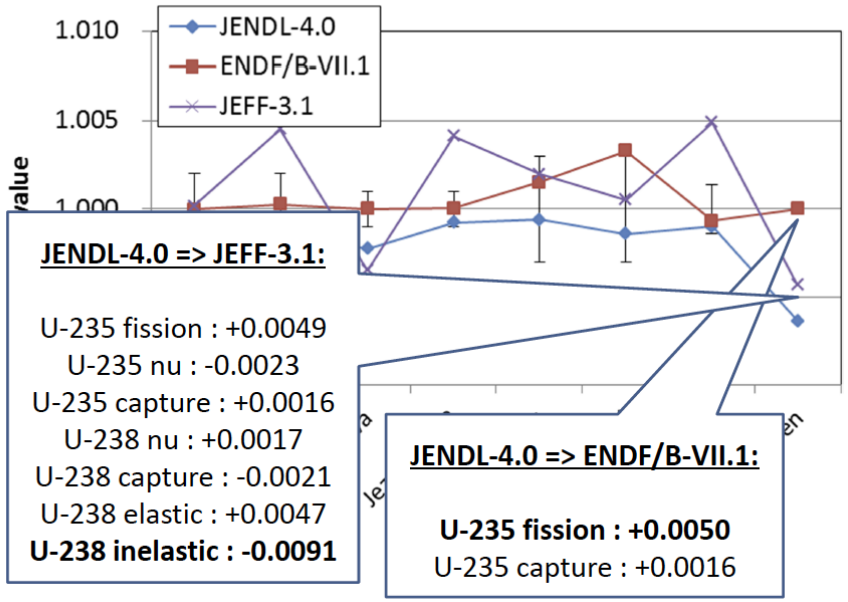
Multiplicity Dependent –PFNS Can be Added to ENDF, for SNM Detection Applications. Example from Vogt (LLNL)



Differences in Reasons for 238U,235U Criticality in Bigten

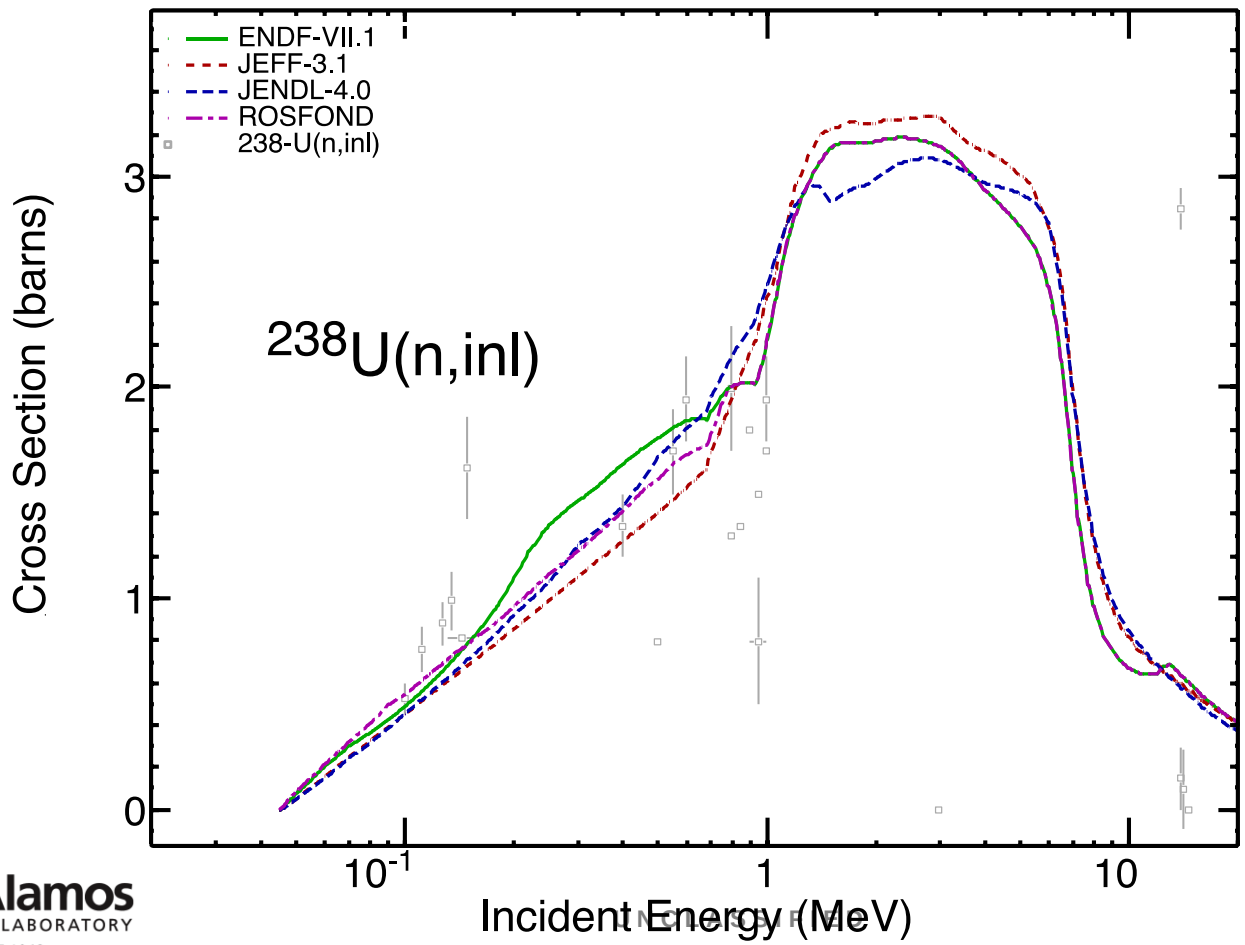
Japanese analysis

Very small fast systems & BigTen



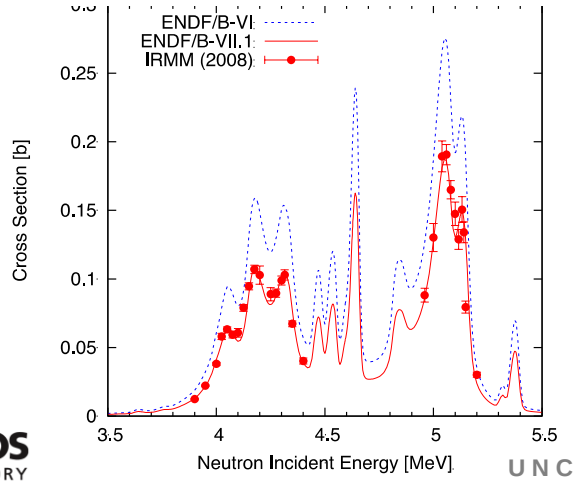
Inelastic & elastic are modeled very differently. (PFNS effect would be larger except all evals use a similar approach)

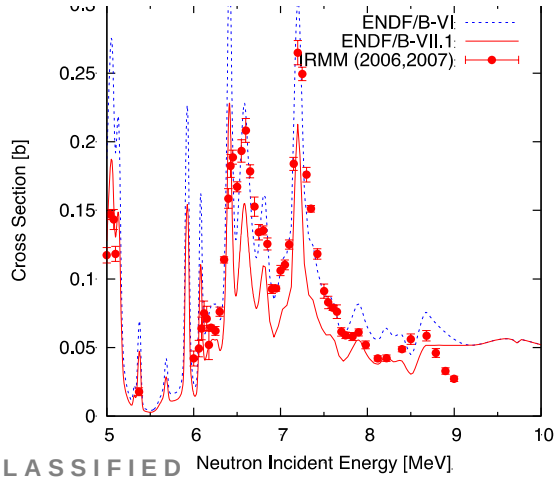
238U Inelastic Scattering: Smaller Discrepancies Here Compared to 239Pu



^{16}O. Much Work is Needed, As We Seek To Maintain Good Criticality and Transmission Performance

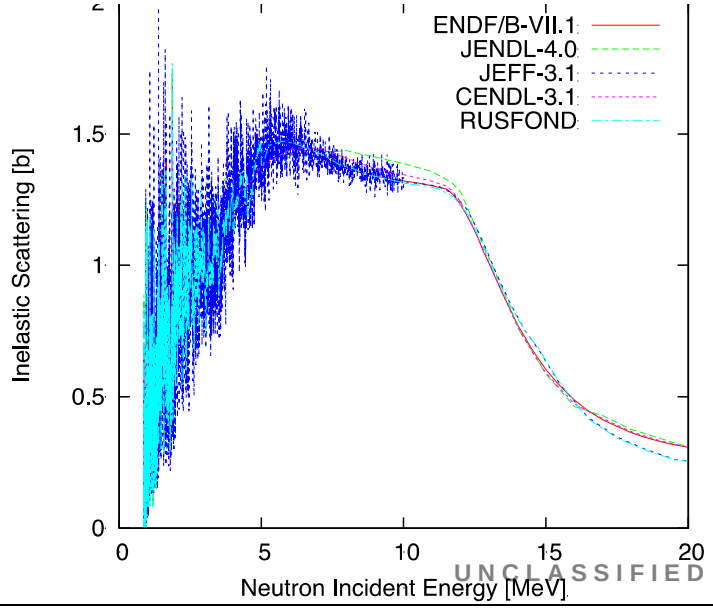
Reaction channel	Issues
Capture	JEFF will likely want to update to the JENDL/ENDF higher energy capture cross section that includes resonance effects for nuclear astrophysics applications
Inelastic, xs and ang dist	?
Elastic, xs and ang dist	At thermal the scattering evaluations differ from Dilg/Mughabghab. In general, it would be good to upgrade the present KAPL-LANL hybrid evaluation.
(n,a)	ENDF, JEFF, and JENDL are similar (adopted ENDF; in JENDL case below 6.5 MeV). ENDF looks good up to 6 MeV, though Hale has been considering changes. At higher energies the data suggest a change is needed (away from Davis data).





^{56}Fe.

Reaction channel	Issues
Resonances	JEFF, JENDL from Frohner's work, ENDF use an earlier Perey and Perey analysis
Inelastic, xs and ang dist	JEFF has resonance effects up to 10 MeV. Also, note that experiments at Ohio University suggest significant changes to the total nonelastic cross section > few MeV (21% at 6.2 MeV increasing to 35% at 10.8 MeV)
Elastic, xs and ang dist	?
(n,a)	ENDF uses some updates based on Kunieda-Kawano's analysis of LANSCE data



Note that fast reactor simulation projects, eg SG33, Commara, JAEA ADJ, have pointed to the large sensitivity to iron inelastic scattering

Creating a New B-VIII Library … Lessons Learned

- **Labs must finalize submissions well before the release date, to allow data testers time, and allow for changes based on testing**
  - 1 year ahead, not months ahead
  - VDM: “last minute changes unacceptable”
  - We need an in-house large-scale automated criticality testing capability
- **Labs should test data themselves before submitting**
  - Understand and document changes in performance
  - Avoid problematic files where errors are found by others
  - We need more data testing & validation. BNL tools are enabling this.
- **First, do no harm. Only make changes when well motivated & defensible**

Quality: ENDF/B-VII is a product that the nuclear science & technology has widely adopted because of its quality, & the intellectual content it contains

We are the trusted providers of nuclear data – keep it this way!