LLNL Evaluation Work in FY09

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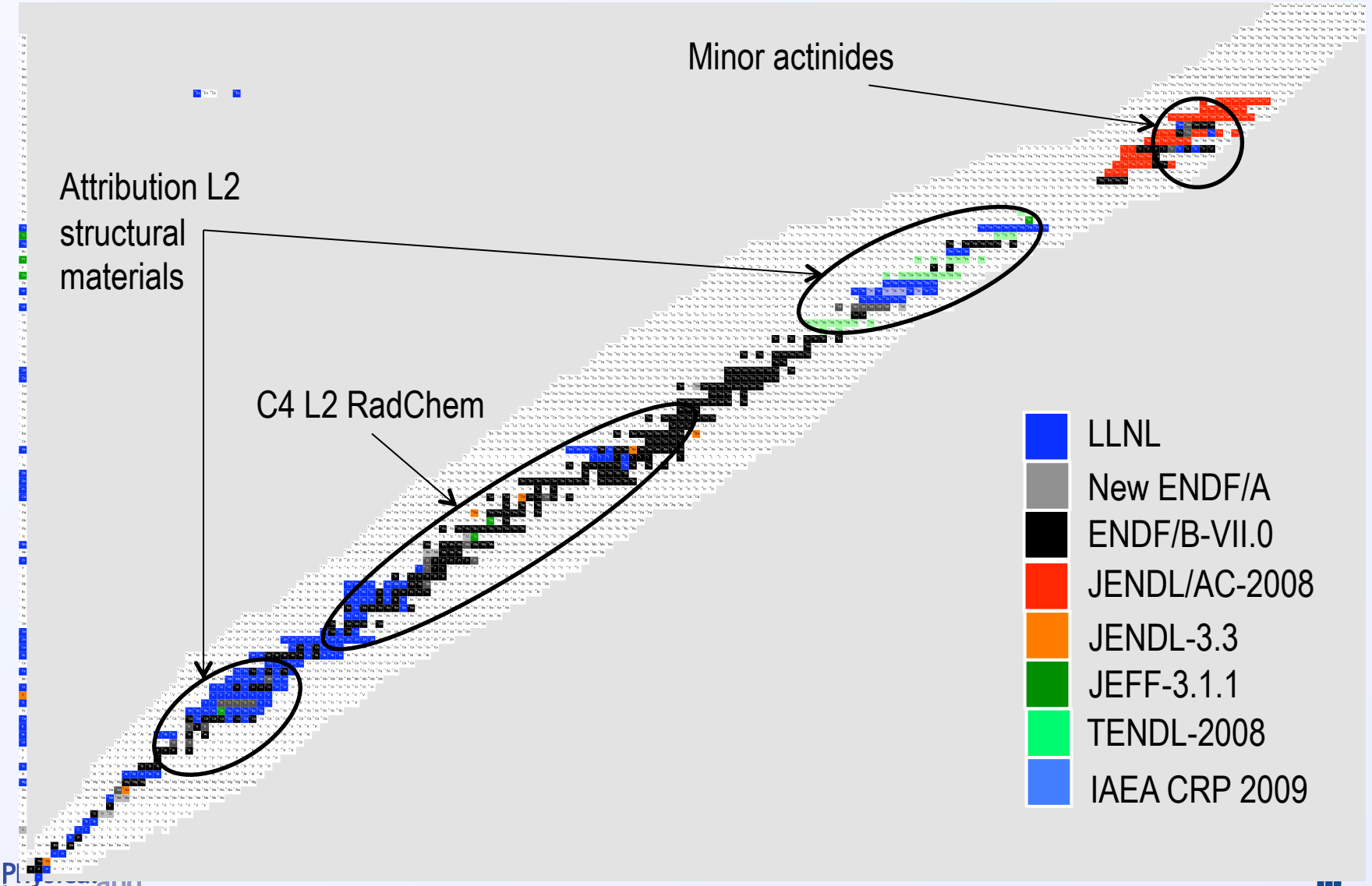
CSEWG Meeting, 11/3/2009

Lawrence Livermore National Laboratory

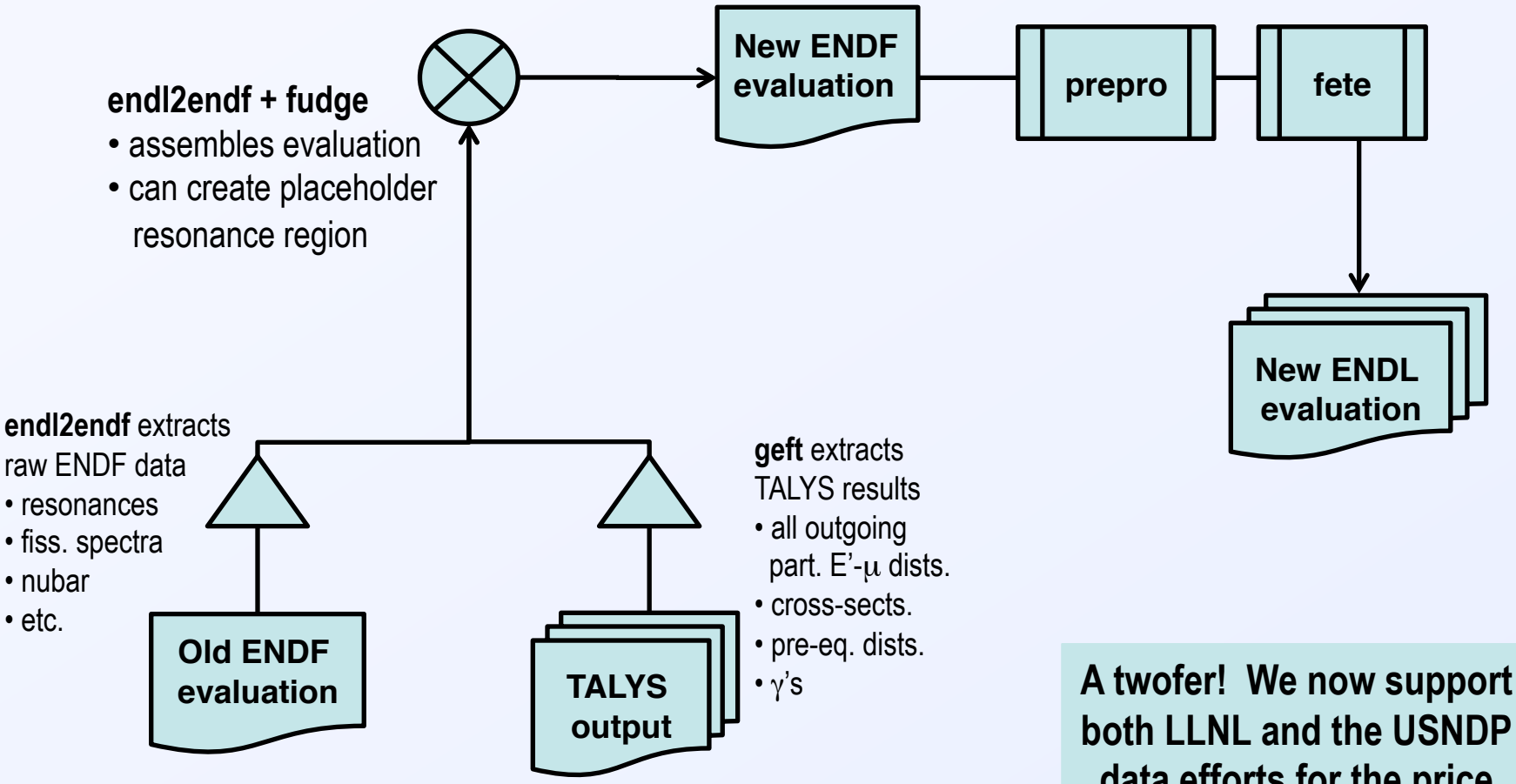
We want to have ENDF/B & ENDL libraries synchronized to greatest extent possible

- LLNL maintains its own internal nuclear data library: ENDL
  - Traditionally not updated frequently: 110 isotopes in neutron sublibrary, last minor revision in 1994
  - ENDL2008 changed this: 526 isotopes in neutron sublibrary, 61% from ENDF/B-VII.0
  - ENDL2009 continues this as will ENDL2010
- LLNL's evaluation capabilities languished between 1995 – 2005
- ENDL & ENDF are (hopefully) asymptotically approaching one another
  - Release cycles very different (ENDL ~ yearly, ENDF ~ every 3-5 years)
  - LLNL customers needs differ from broader nuclear data community
  - Formats & processing very different
    - LLNL moving from legacy internal formats & codes to XML, OOP formats & infrastructure (see B. Beck's talk)
    - ENDF still uses legacy formats and processing must support it
    - ARRA-funded project to update ENDF

In ENDL2009, we aim to choose the best available evaluations, whatever the source is



Our new evaluation procedures produce *complete* ENDL and ENDF evaluations

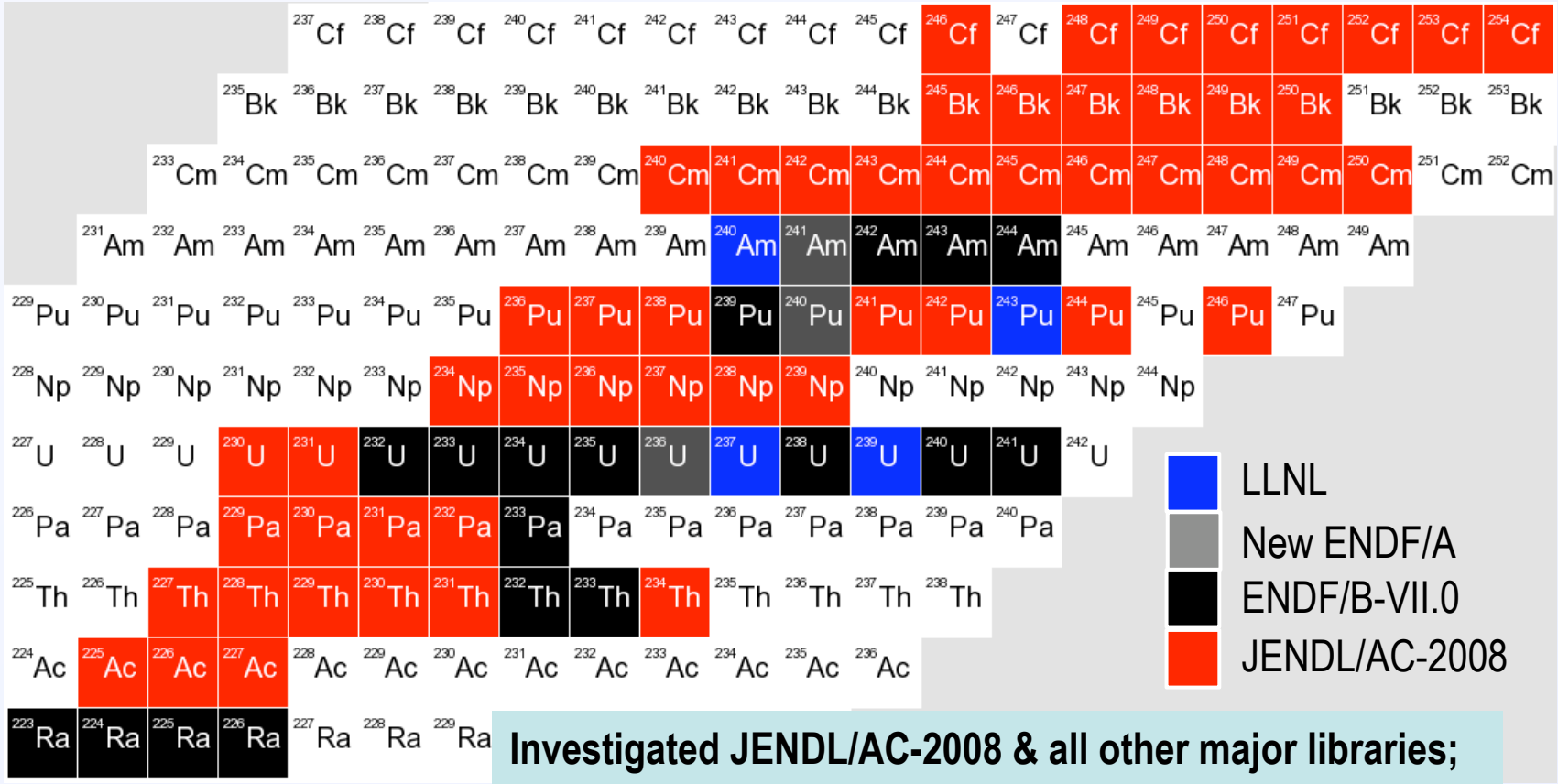


A twofer! We now support both LLNL and the USNDP data efforts for the price of one

Outline for the talk

- Background
- **Actinides**
  - **JENDL/AC-2008 review**
  - **240Am**
  - **239U**
- Structural materials
- Other Misc. evaluations

Results from review the JENDL Actinoid 2008 (JENDL/AC-2008) Library

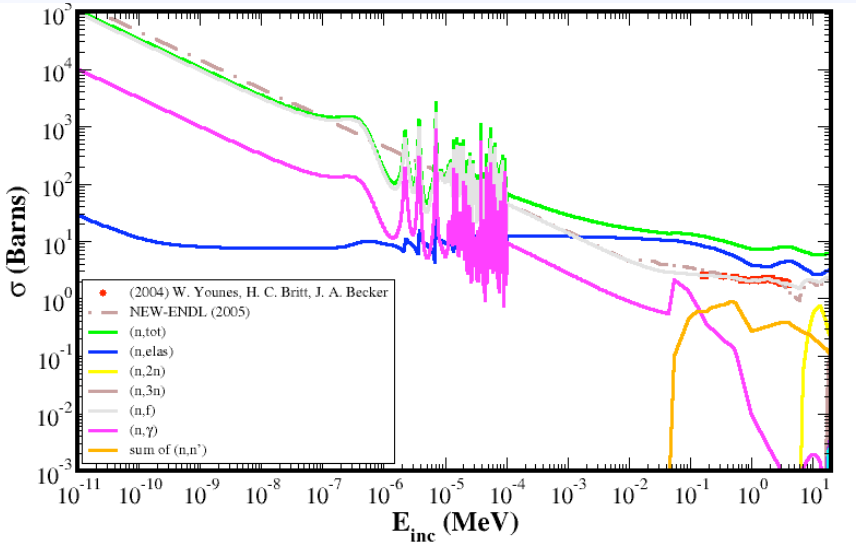


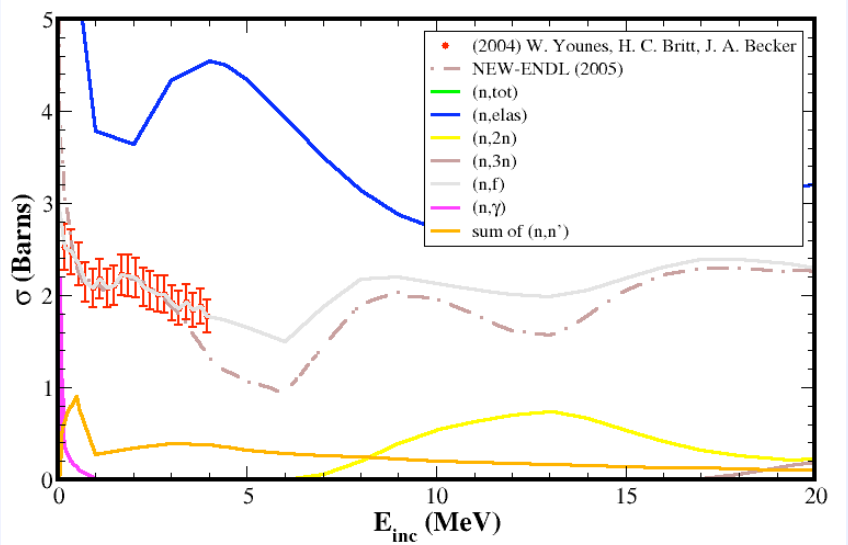
Investigated JENDL/AC-2008 & all other major libraries; made recommendations based on:

- **Visual inspection of cross section plots**
- **χ^2 compared to cross section data**
- **Scope and quality of systematics when no data**

Technical report LLNL-XX-XXXX, will upload recommendations to ENDF/A

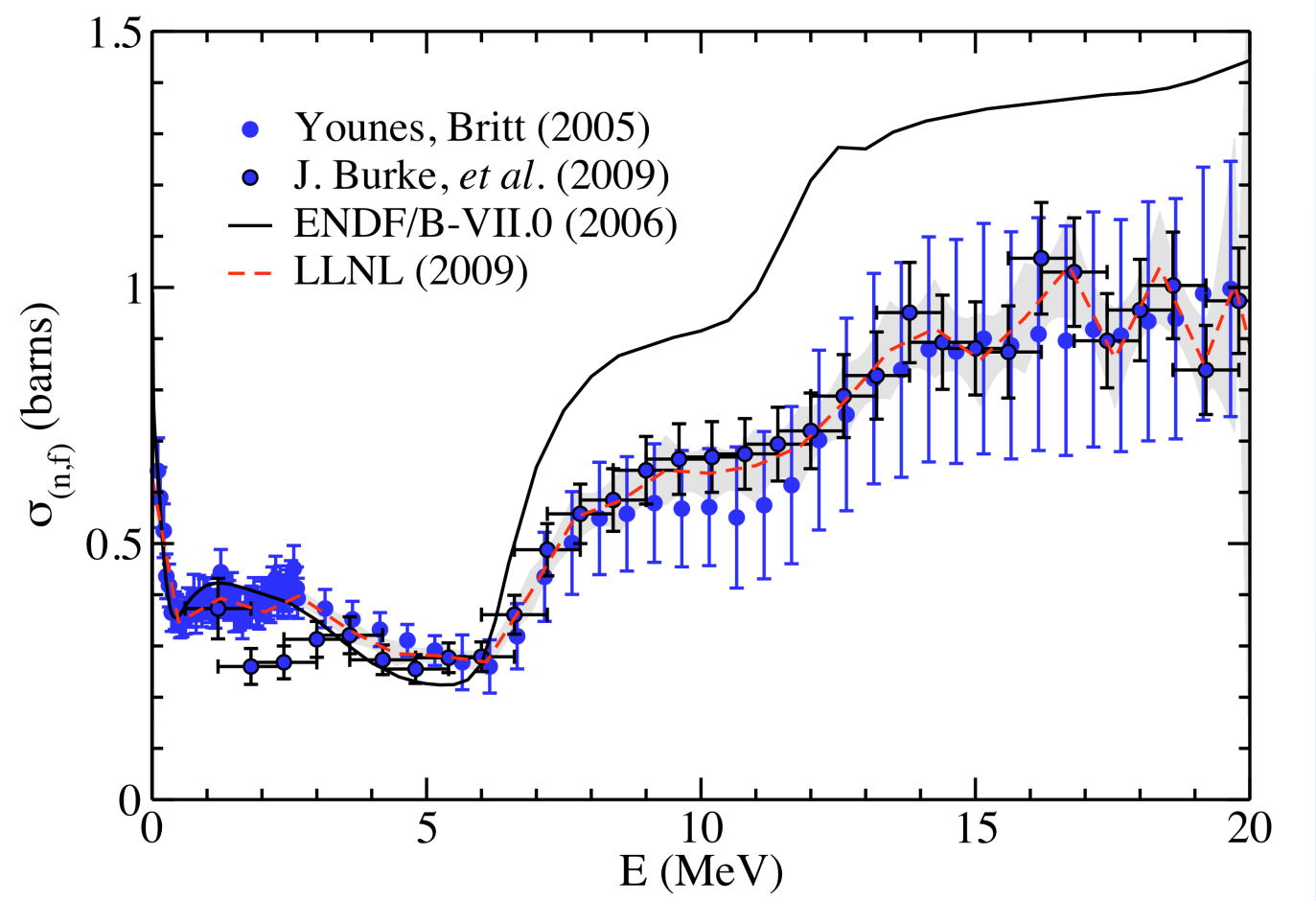
^{240}Am evaluation: requires further modification before ready for ENDF/B-VII.1





- Used TALYS + `geft` + `endl2endf`
  - Soukhovitskii, Chiba et al. OMP
  - RIPL levels, masses, etc.
- Resonance data, ν and fission spectrum from ^{242}Am evaluation in ENDF/B-VII.0
  - *Resonances from JENDL/AC-2008 better, we should adopt those*
- Everything else from TALYS:
  - σ's
  - spectra
  - γ's
  - angular distributions
- We tuned cross sections:
  - Swap in Younes, Britt (n,f) evaluation based on surrogate (t,pf)
  - *Attempted to match σ's onto resonances: should redo w/ JENDL/AC-2008 resonances*

Burke *et al.* performed surrogate measurement of ^{239}U(n,f), so we re-evaluated ^{239}U, folding in Younes & Britt (n,f) evaluation

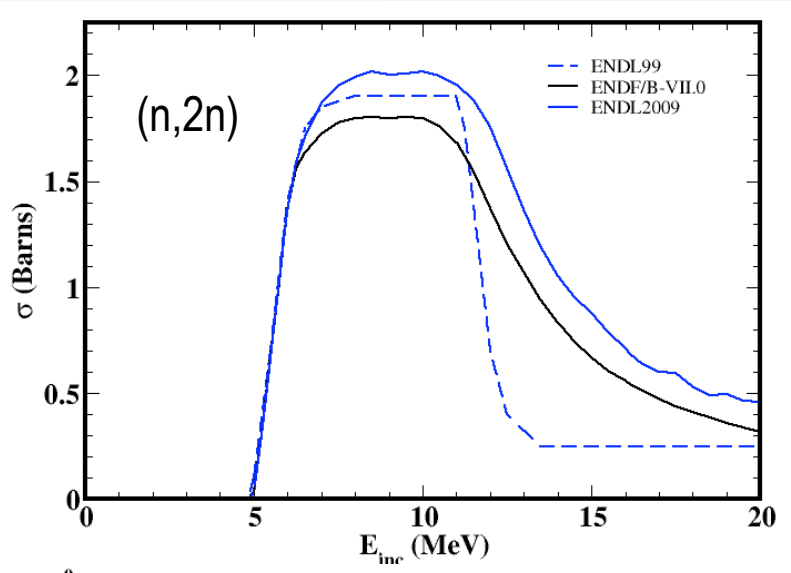


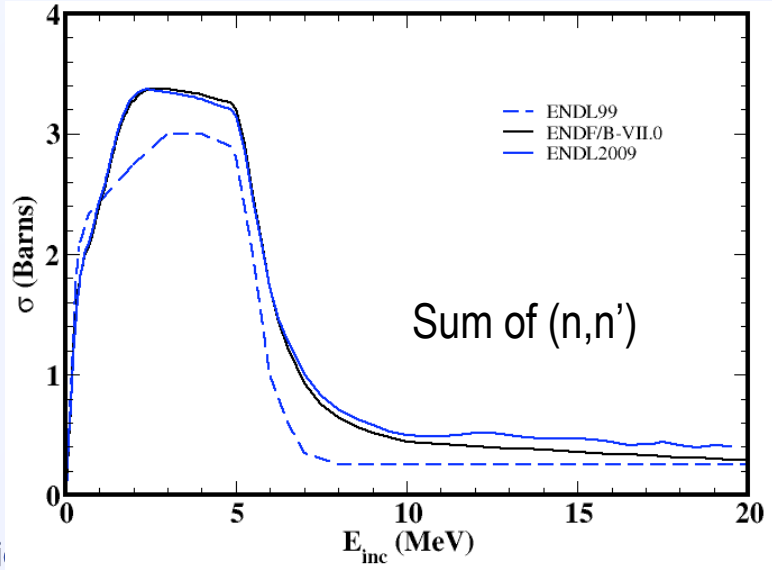
Fit folds in uncertainties from three classes of surrogate measurements: (t, pf), (^{3}He, xf) and (^{18}O, ^{17}O)

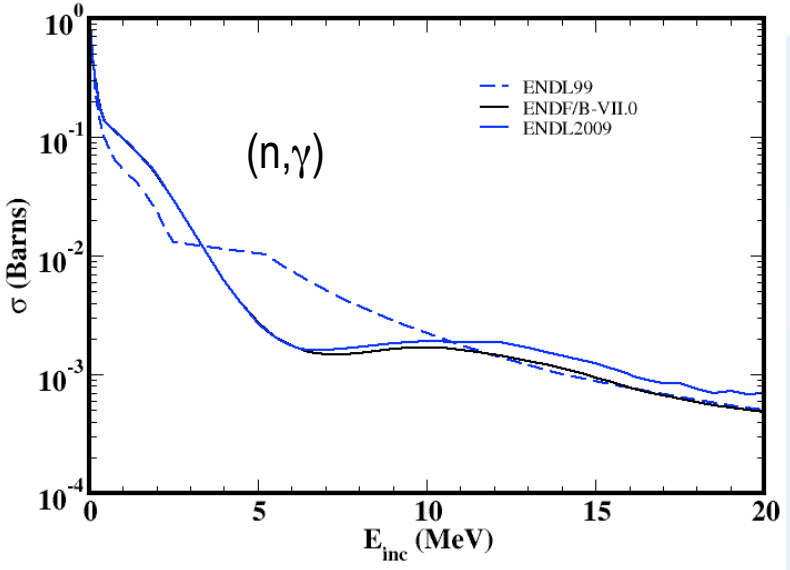
We have changed the fission cross-section, so we must correct the ENDF/B-VII.0 cross-sections too

- **Assuming:**
  - **Weisskopf-Ewing limit**
  - **Compound elastic contribution negligible**
- **Then the correction is a simple rescaling:**

$$\sigma_{\text{new}} = \sigma_{\text{old}} \times \frac{\sigma_{\text{rxn}} - \sigma_{\text{fixed fission}}}{\sigma_{\text{rxn}} - \sigma_{\text{bad fission}}}$$





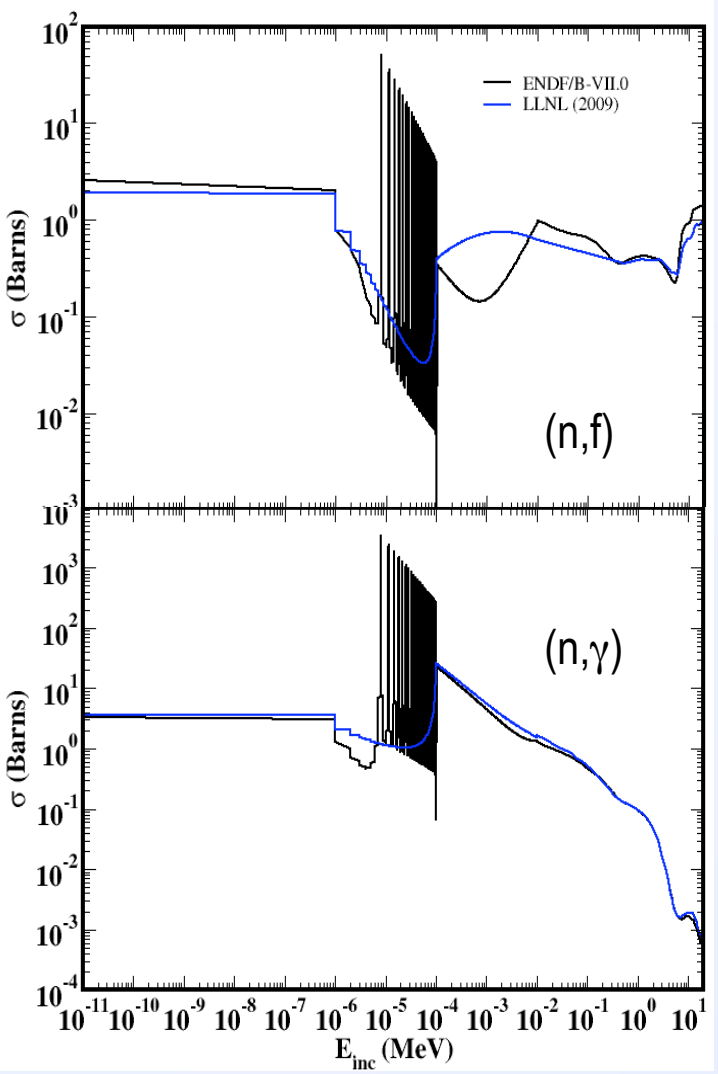


The original ^{239}U resonances required several fixes since they were a copy of the ^{237}U resonances

- RRR was "picket fence"
- URR average parameters matched to "picket fence"
- J^{Π} set to ^{237}U values g.s. of ^{237}U is $\frac{1}{2}^{+}$
- Changing to ^{239}U J^{Π} made things worse (g.s. of ^{239}U is $5/2^{+}$)
- Matching onto high energy (n,f) looks scary

Use URR for all resonances, match averages to high energy cross-sections and thermal σ values from Mughabghab

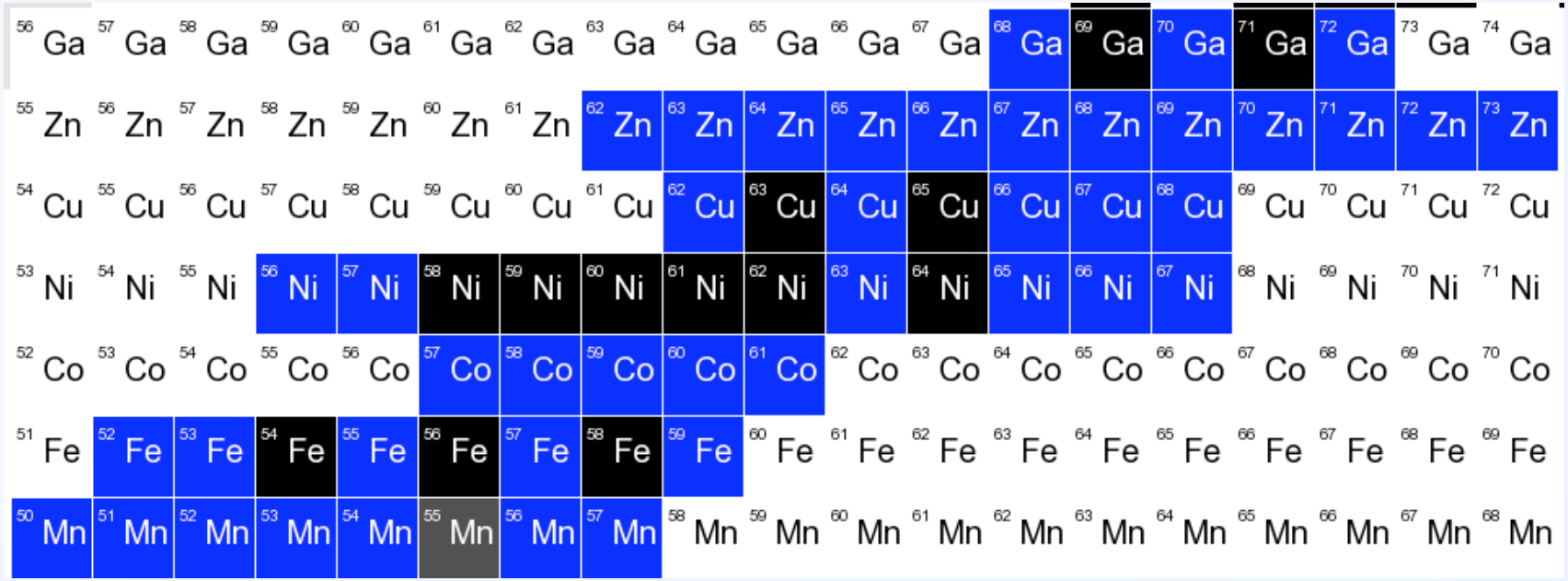
Channel	Therm. σ (barns)	Therm. σ (barns) Mughabghab	Res. Int. (barns)
(n,el)	21.32		199.9
(n,γ)	22.16	22 ± 5	50.5
(n,f)	13.97	14 ± 3	19.0



Outline for the talk

- Background
- Actinides
- **Structural materials**
  - **Zn**
  - **Al**
  - **57Fe**
  - **59Co**
  - **Ni**
  - **Ta**
  - **Re**
  - **Pb**
  - **W**
- Other Misc. evaluations

Light structural materials (FY08 Attribution L2 Milestone)



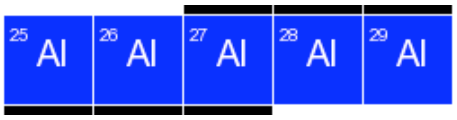
Ian Thompson
(Attrib. structs.)

Neil Summers
(USNDP POC, tool devel.)

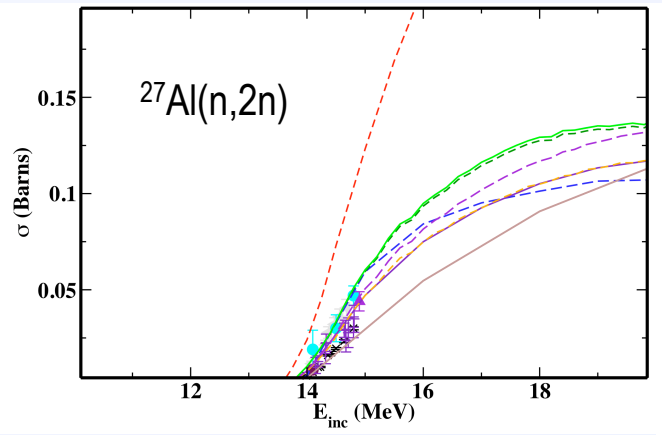
Rob Hoffman
(systematics, RadChem)

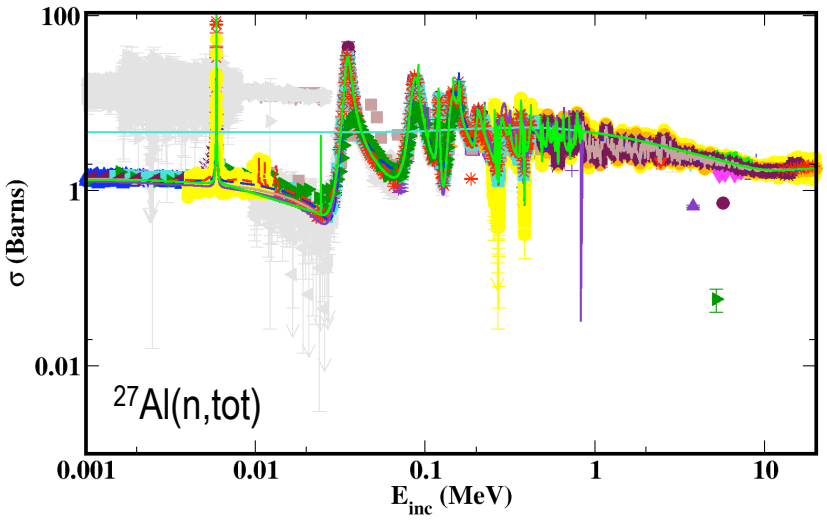
- FY08, added many new evaluations
  - Co & Zn packed in ENDF format
  - others available if interested
- FY09, added 3 Al evaluations
- New assemblies allow us to test

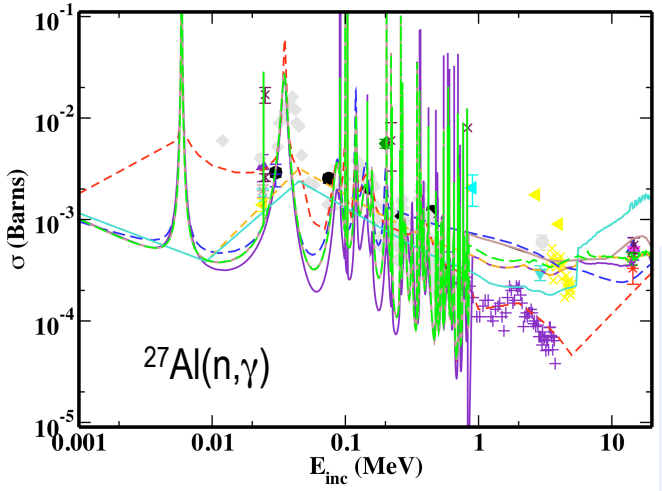
Al (Z=13)

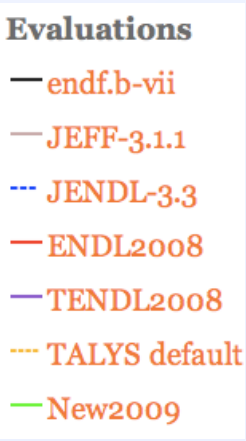


- Stable ^{27}Al, want $^{25\text{-}29}$Al
- ^{27}Al: Resonance parameters defined up to 1 MeV, but still slightly fluctuations up 10 MeV.
- Resonances (to 1 MeV) from ENDF/B.VII
- Large (n,γ) data disagreements above 1 MeV!
- Large (n,tot) data disagreements below 20 keV!
- Final result is green line; use green-line Talys default also for unstables (without resonances).
- Crits. & pulsed sphere tests in Descalle's talk





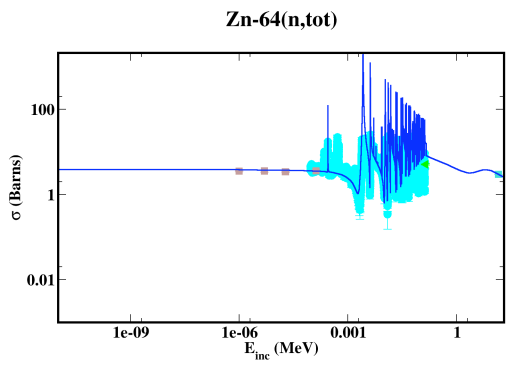


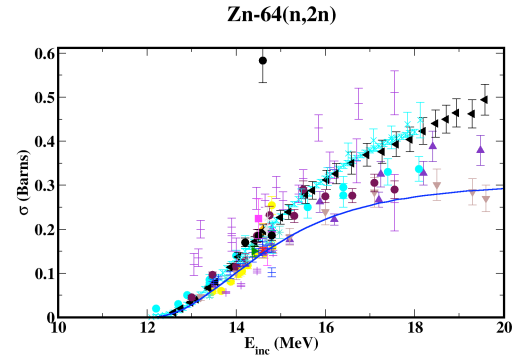


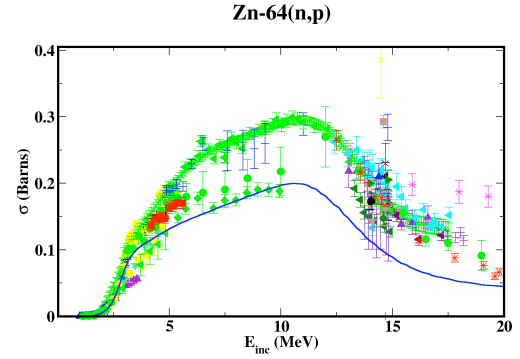
We are submitting this to ENDF/A for (we hope) inclusion in ENDF/B-VII.1

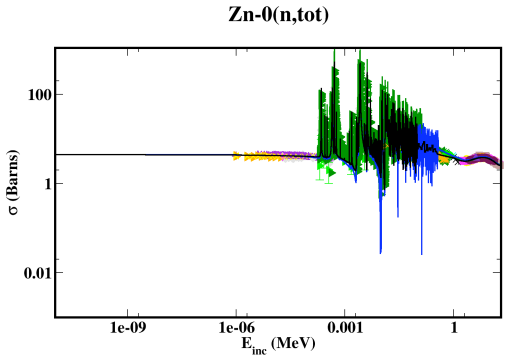
Zn (Z=30)

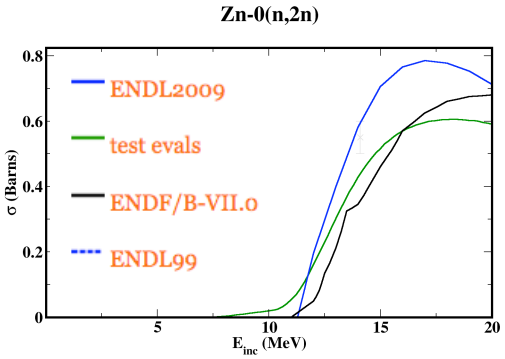
- We developed isotopic evaluations for A=62-73
- Used TALYS calculation:
  - systematics developed by Hoffman for level densities, gamma ray str funcs
  - Koning-Deleroche OMP
- ^{nat}Zn ENDF resonances disassembled to fill out stables
- Cross sections *not fitted*, data needs detailed sorting out (e.g. (n,2n) to right)
- Reassembled natural eval. Compares well to ^{nat}Zn eval.
- Performs well in crits (see Descalle talk)
- Will generate tech report detailing evaluation(s)



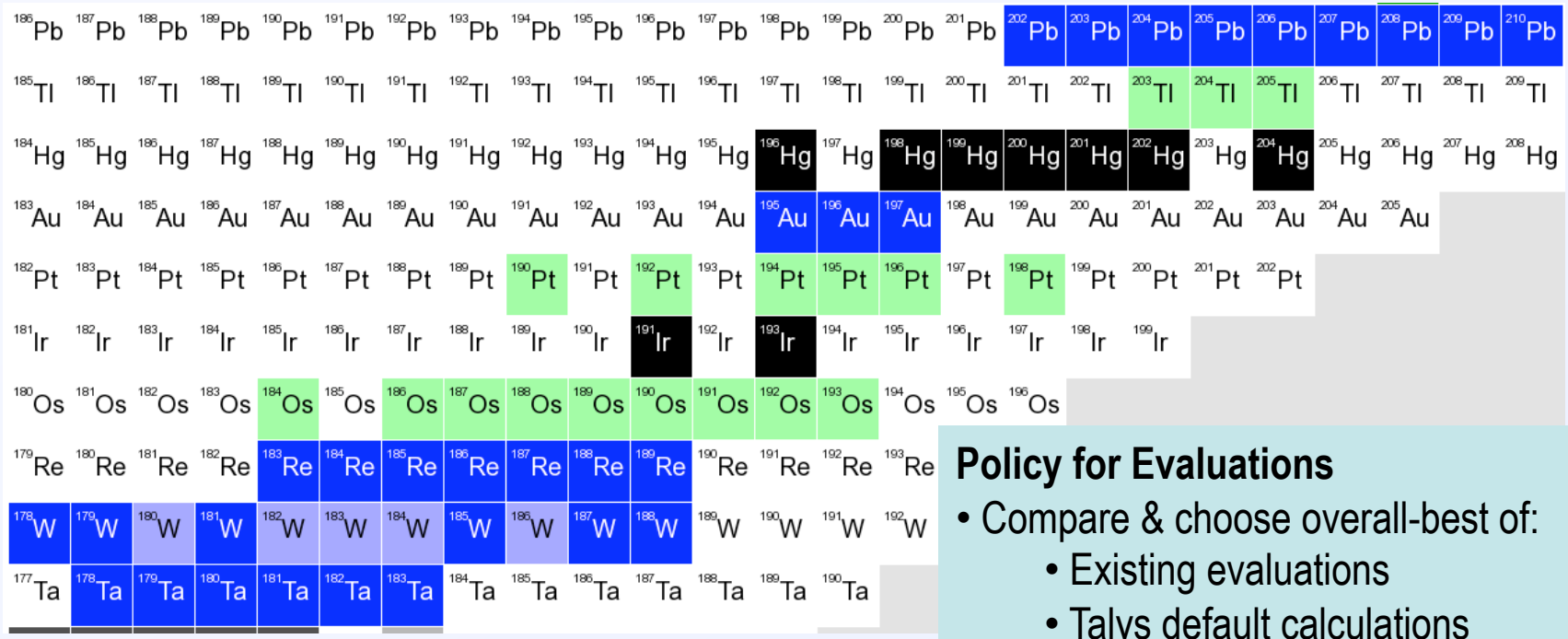


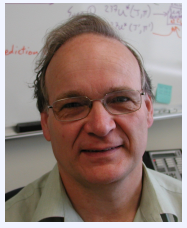






Heavy structural materials (FY09 Attribution L2 Milestone)





Ian Thompson (Attrib. structs.)

Neil Summers (USNDP POC, tool devel.)

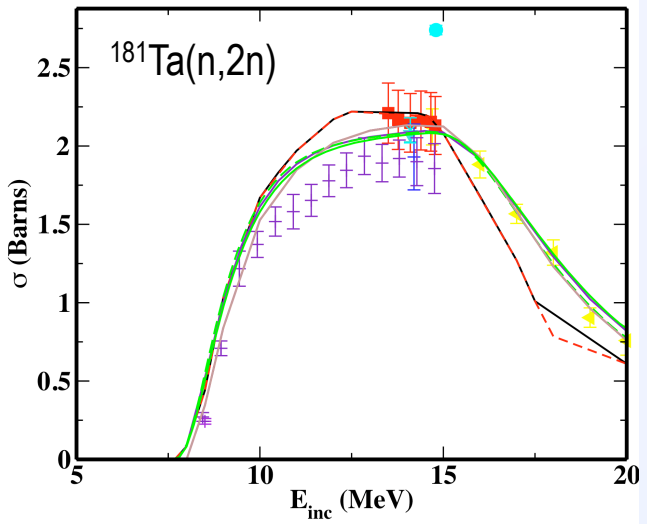
Dave Brown (project POC, tool devel., actinides)

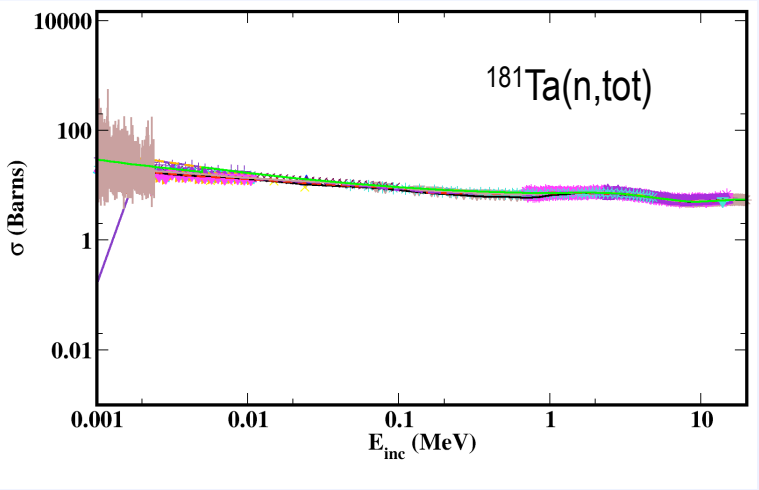
Policy for Evaluations

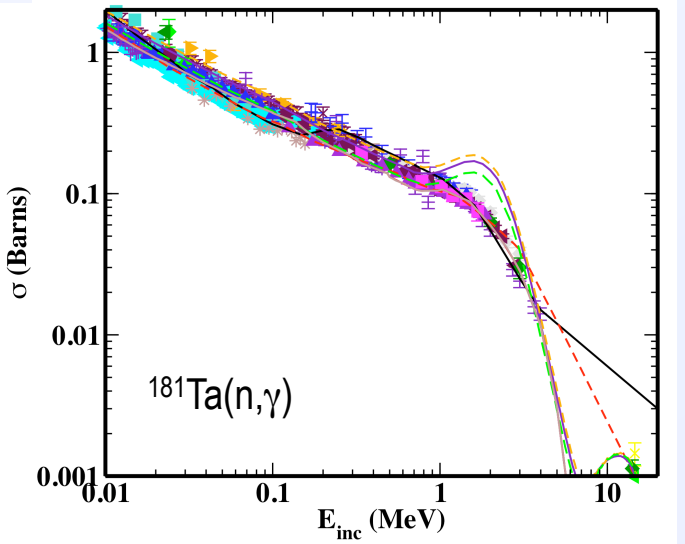
- Compare & choose overall-best of:
  - Existing evaluations
  - Talys default calculations
  - Talys with some tuned params.
  - Focus on largest c.s., then (n,γ)
- If choosing Talys run, use best resonances from other evaluations.
- No Isomers: only initial gs; final states summed.

Ta (Z=73)

- Only ^{181}Ta is stable, want $^{178\text{-}183}$Ta.
- (^{180}Ta has isomer state at 10^{15} years!)
- ^{181}Ta: resonance info up to 2 keV.
- No best modern evaluation for (n,γ)
- Use Talys default also for unstables
- Pulsed sphere results in Descalle's talk



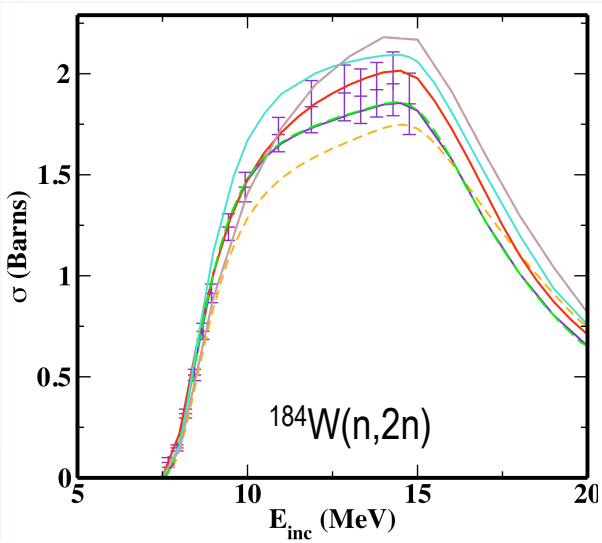


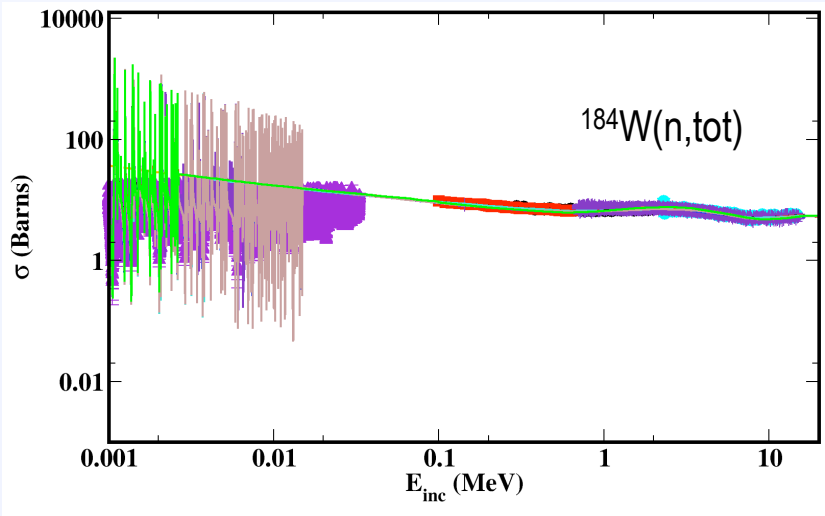


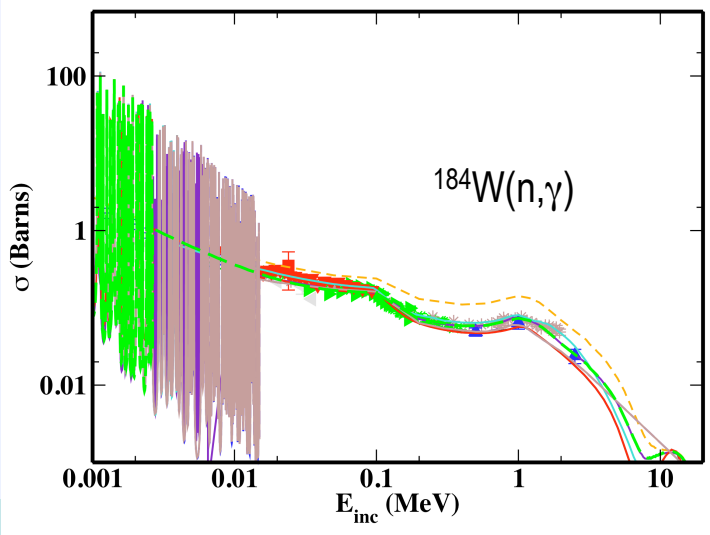
We are submitting these to ENDF/A for (we hope) inclusion in ENDF/B-VII.1

W (Z=74)

- Stable $^{180,182\text{-}4,186}$W, want also $^{178\text{-}9,181,185,187\text{-}8}$W.
- The recent IAEA evaluation of stable W is clearly the best for all of these, including resonances.
- The default-talys curves are plausible for stable W; show plots for ^{184}W.
- So, use default talys for the unstable isotopes.
- Show pulsed sphere results in Descalle's talk



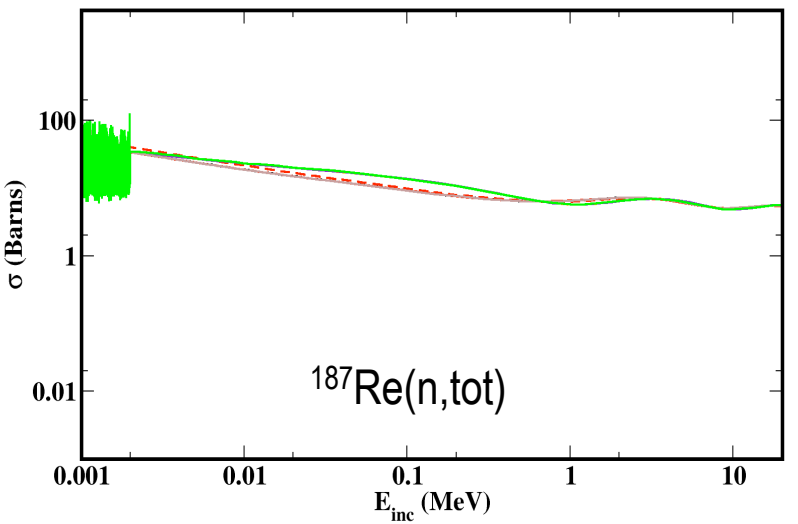




We are submitting the unstables to ENDF/A for (we hope) inclusion in ENDF/B-VII.1, we recommend the IAEA W evals for the stables

Re (Z=75)

- Stable ^{185,187} Re, need $^{183\text{-}9}$Re.
- Very little (n,tot) data for any isotope.
- For ^{185,7}Re, after reducing TALYS default Γ_γ TALYS is ok.
- So use for unstable isotopes too.



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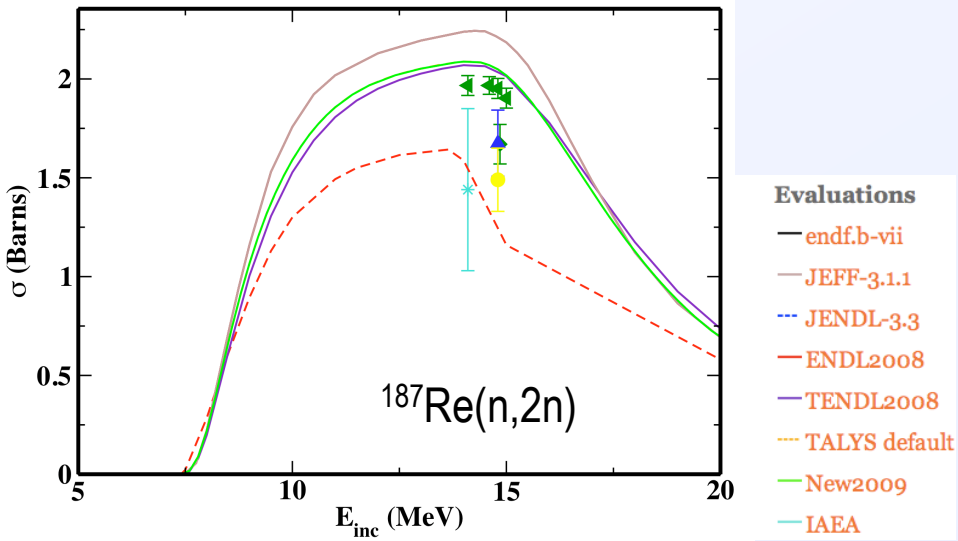
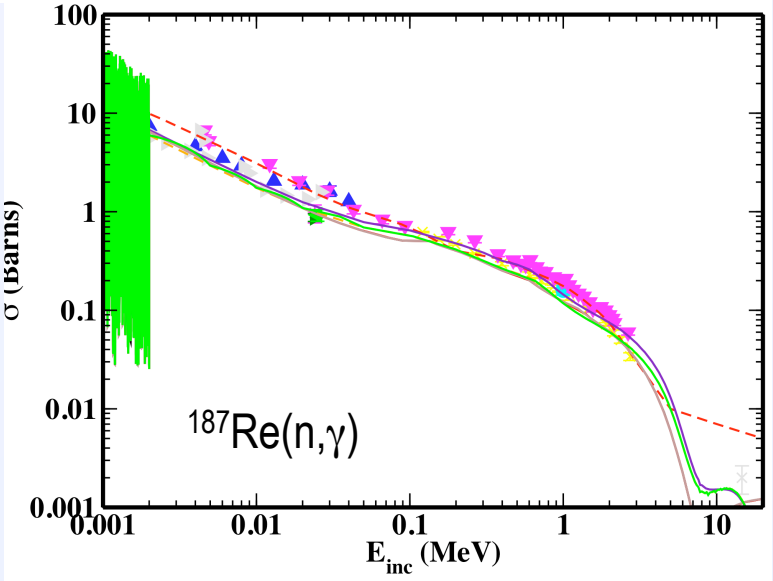




Other evaluations we've performed, but aren't ready to submit to ENDF/B-VII.1

- 204,206,207,208Pb
  - Ours is tuned TALYS calc with ENDF/B-VII.0 resonances (they extend very high due to closed shell)
  - Poor performance in pulsed spheres
  - k_{eff} systematically high in critical assemblies
- 57Fe: not different enough
  - Ours is merger of NRG evaluation & ENDF/B-VII.0 resonances
  - NRG (using TALYS) evaluation nearly identical to ENDF/B-VII.0 (using GNASH)
  - Performance in crits & pulsed spheres nearly identical
- 59Co: needs fix
  - Ours is tuned TALYS calc w/ ENDF/B-VII.0 resonances
  - Recently discovered bug: resonance smooth background wrong
  - Abysmal performance in activation ratio tests
  - k_{eff} systematically high in critical assemblies

Outline for the talk

- Background
- Actinides
- Structural materials
- **Other Misc. evaluations**
  - **Background**
  - **Au**
  - **Xe**
  - **As**
  - **Ar**

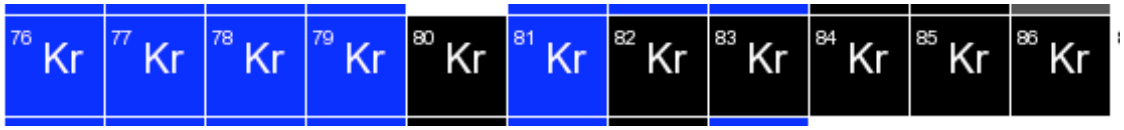
Nuclear data required for diagnostics (Campaign 4 L2 Milestone)

- Nuclei of lightest known isotope offer a unique (n,2n) diagnostic
  - Network of nuclei with multiple (n,2n) reactions as well as (n,γ)
  - In principle, fewer problems with background as the reaction products are radioactive and not present in nature
- This presents a challenge as data is limited and only available, if at all, for the first nuclei and none for the secondary products
  - We must rely on theoretical methods – TALYS reaction code
  - Benchmark where possible
  - Estimate uncertainties due to model inputs
    - Optical potential – reaction cross section
    - Level densities – channel cross sections
    - Pre-equilibrium models (especially knockout)
  - In some nuclei other charge-particle channels are open and must be understood – competition with neutrons

Erich Ormand
(C4 RadChem)

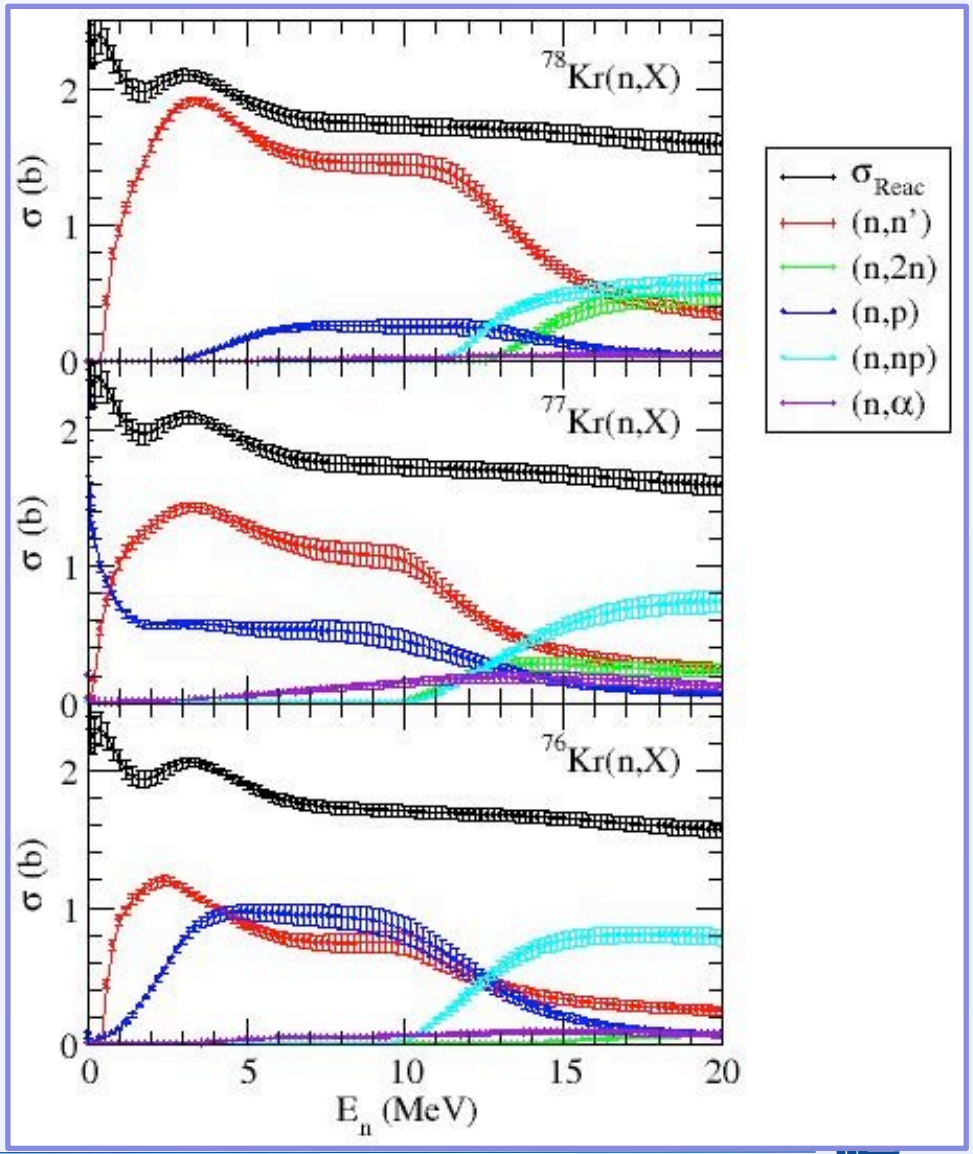
Neil Summers
(USNDP POC, tool devel.)

Kr isotopes



- Small charge-particle channels, neutron channels are reliable
- Resonances taken from ENDF/B-VII.0
- (n,γ) is essentially unchanged from WPEC-23

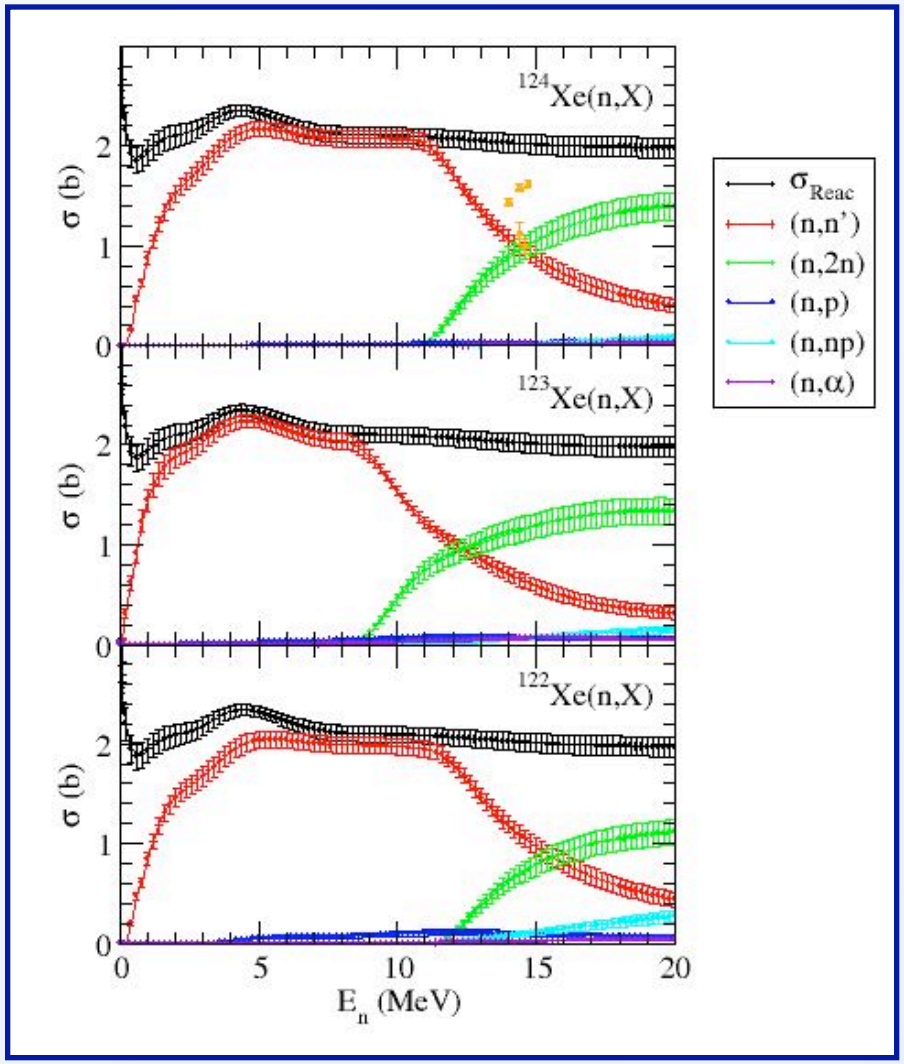
We are submitting this to ENDF/A for (we hope) inclusion in ENDF/B-VII.1



Xe isotopes

- Small charge-particle channels, neutron channels are reliable

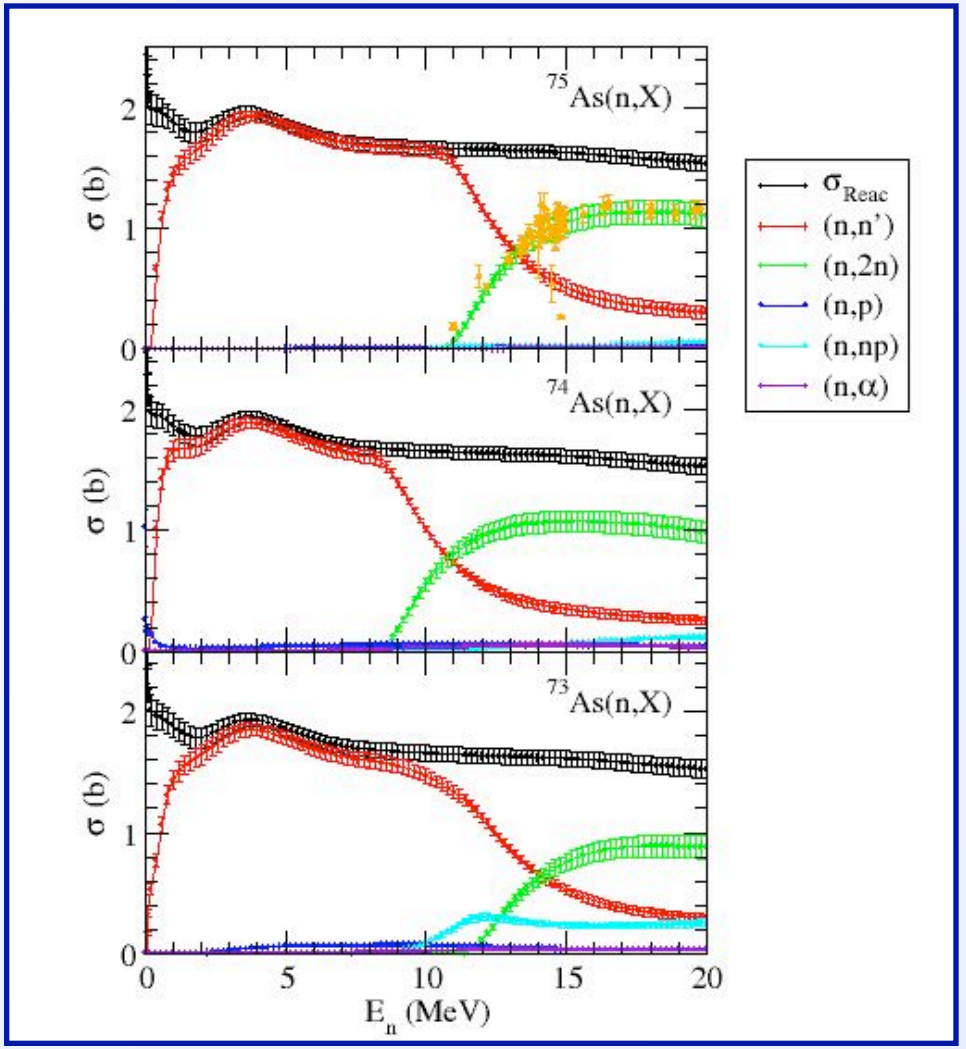
We are submitting this to ENDF/A for (we hope) inclusion in ENDF/B-VII.1



As isotopes

- Abundant (n,2n) data
- Overall agreement with default parameters
- Merged with ENDF/B-VII.0 resonances

We are submitting this to ENDF/A for (we hope) inclusion in ENDF/B-VII.1



Other evaluations we've performed, but aren't ready to submit to ENDF/B-VII.1

- 34,35,36Ar
  - Ours is tuned TALYS calc with ENDF/B-VII.0 resonances
  - Problem discovered with pre-equilibrium model that messed up (n,γ)
  - We will revise and submit for ENDF/B-VII.2 pending fixes in TALYS
- 195,196,197Au
  - Ours is tuned TALYS calc
  - Use ENDF/B-VII.0 resonances, match onto (n,γ)
  - Performs poorly in LLNL pulsed sphere test (see Descalle's talk)
  - We will revise and submit for ENDF/B-VII.2 due to poor performance in pulsed spheres

Summary

- Actinides
  - Submitting recommended JENDL/AC-2008 evaluations (59 minor actinides) for ENDF/B-VII.1
  - Remerge 240Am resonances for ENDF/B-VII.1
  - 237U needs review
  - 239U submitted for ENDF/B-VII.1
- Structural materials
  - Not ready: Pb?, Zn, Co
  - Not worth submitting: 57Fe
  - Submitted for ENDF/B-VII.1: Ta, W, Re
- Other Misc. evaluations
  - Not ready: Ar, Au
  - Submitted for ENDF/B-VII.1: As, Kr, Xe

What's next?

- FY10 L2 milestone to deliver new (n,f) fission neutron spectrum, with covariance (LLNL, LANL)
- MT=458 files re-generated for all actinides in final list (Vogt, Brown)
- Previously listed evaluations
- Thermonuclear reactions (Navratil, Quaglioni, Hale, Brown):