

LLNL Evaluation Work in FY09

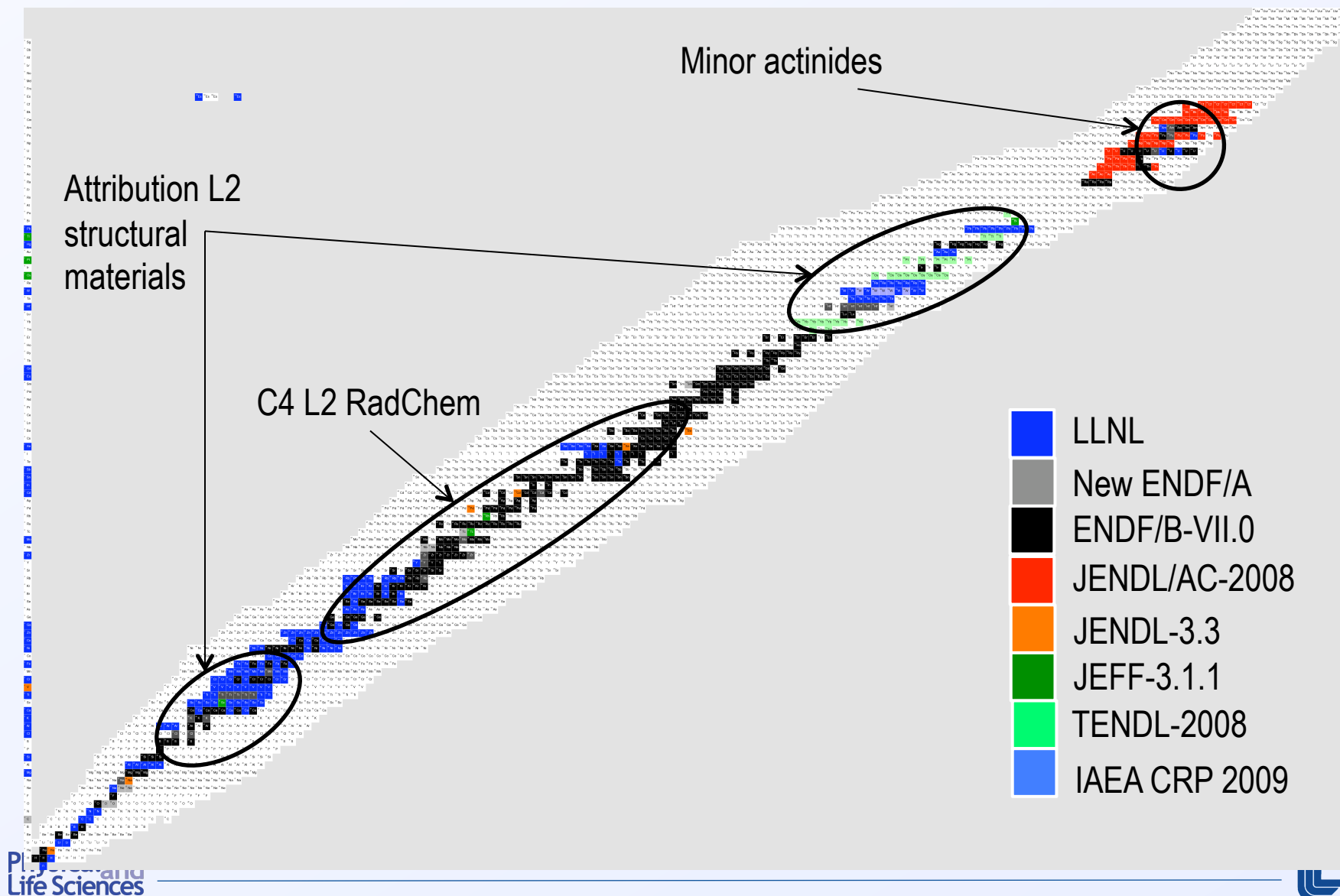
David Brown
CSEWG Meeting, 11/3/2009

Lawrence Livermore National Laboratory

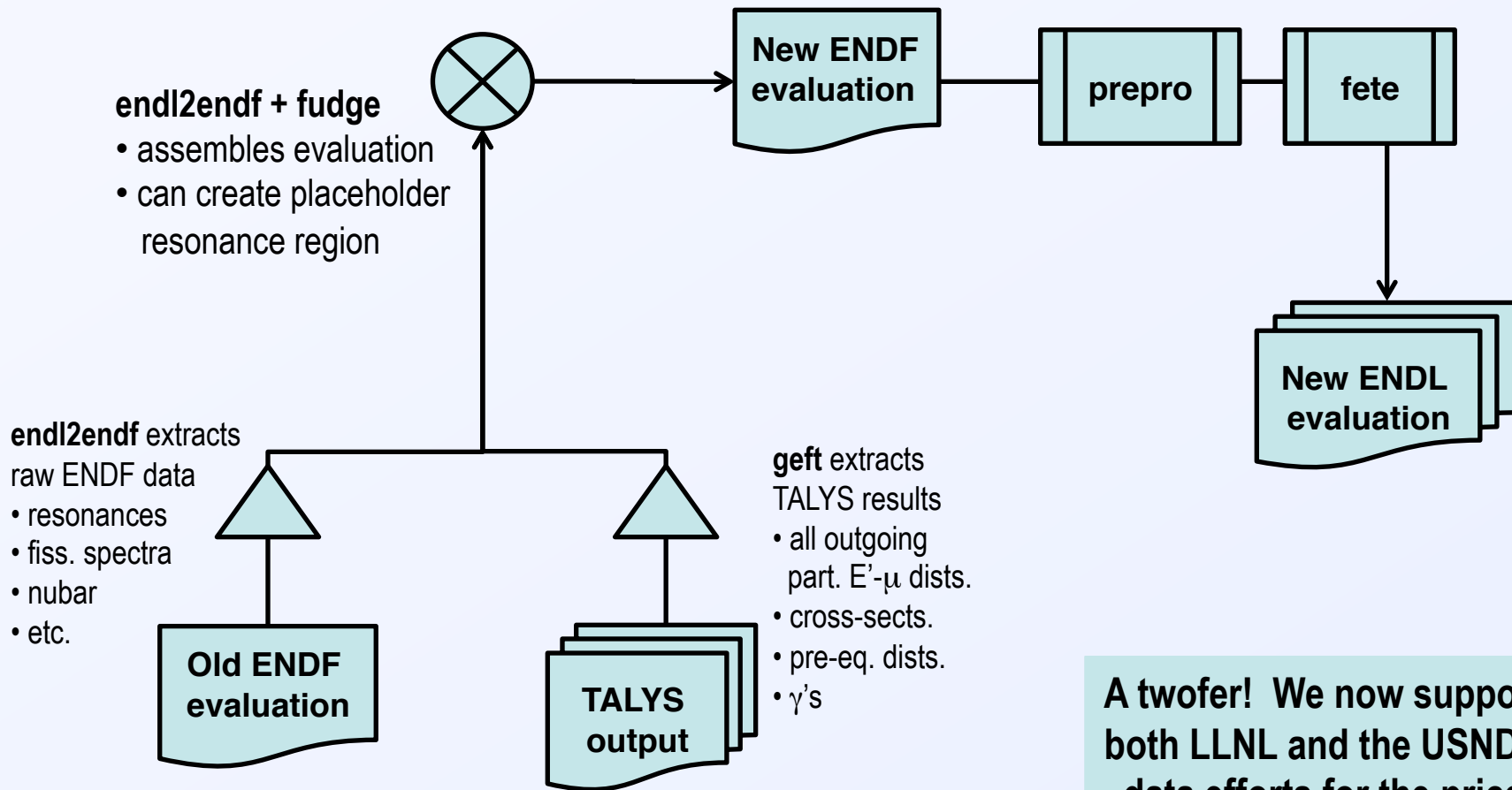
We want to have ENDF/B & ENDL libraries synchronized to greatest extent possible

- 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

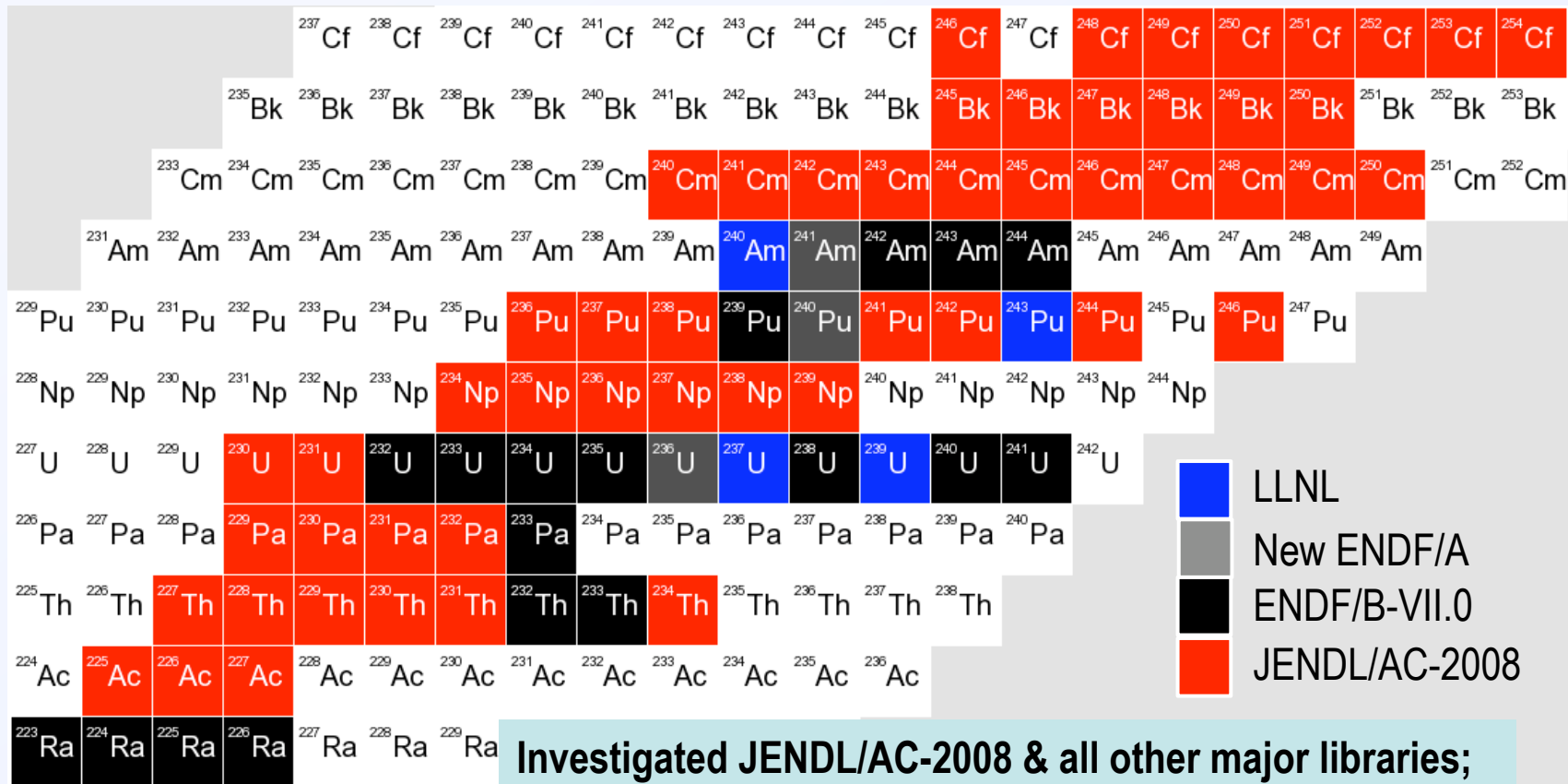


A twofer! We now support both LLNL and the USNDP data efforts for the price of one

Outline for the talk

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

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



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

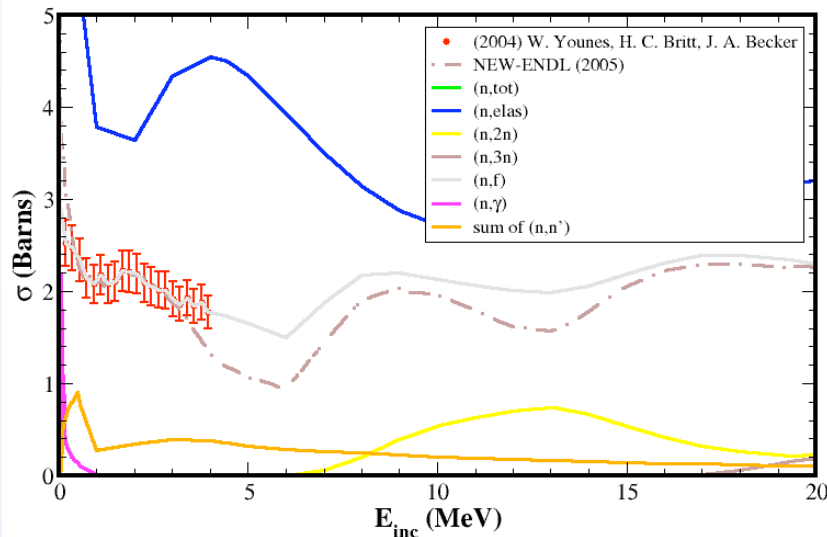
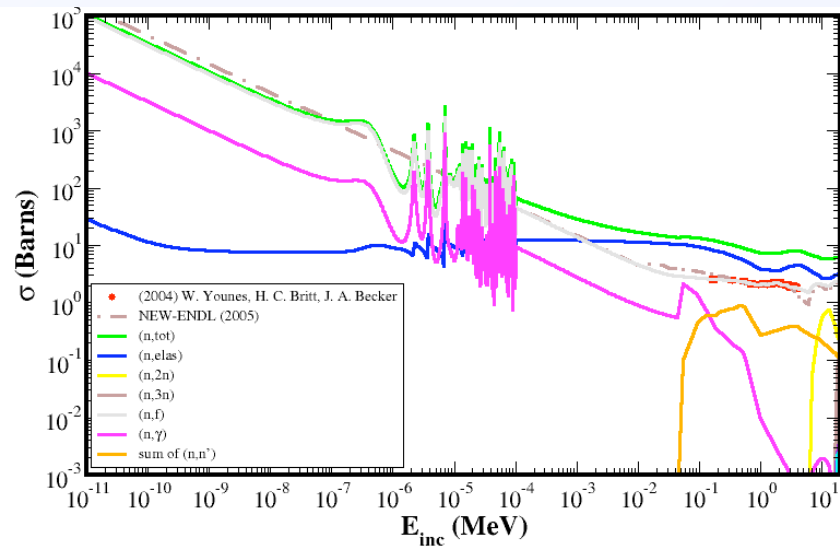
Investigated JENDL/AC-2008 & all other major libraries; made recommendations based on:

Visual inspection of cross section plots

χ^2 compared to cross section data

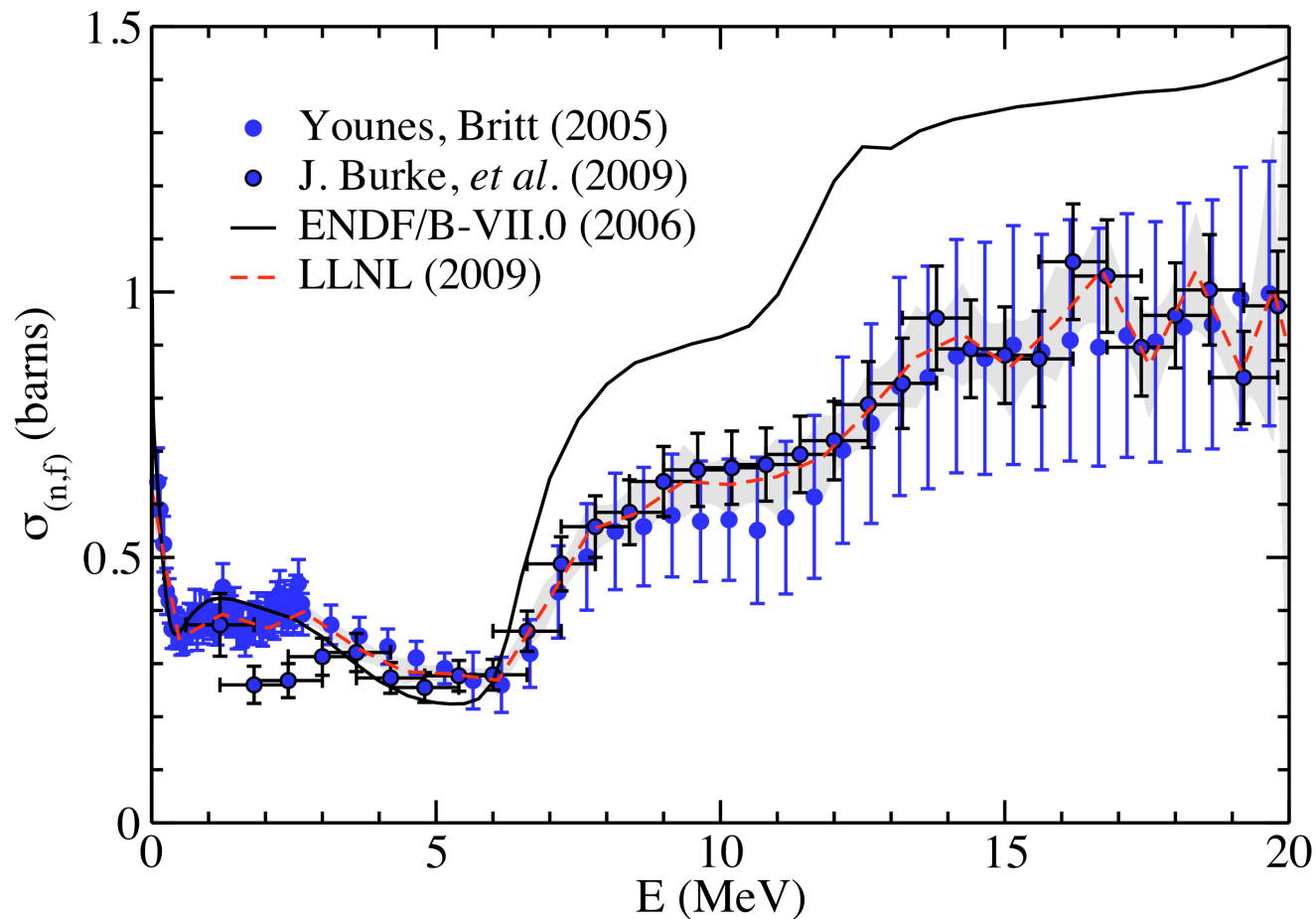
Scope and quality of systematics when no data

²⁴⁰Am 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 ²⁴²Am 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 $^{239}\text{U}(n,f)$, so we re-evaluated ^{239}U , folding in Younes & Britt (n,f) evaluation



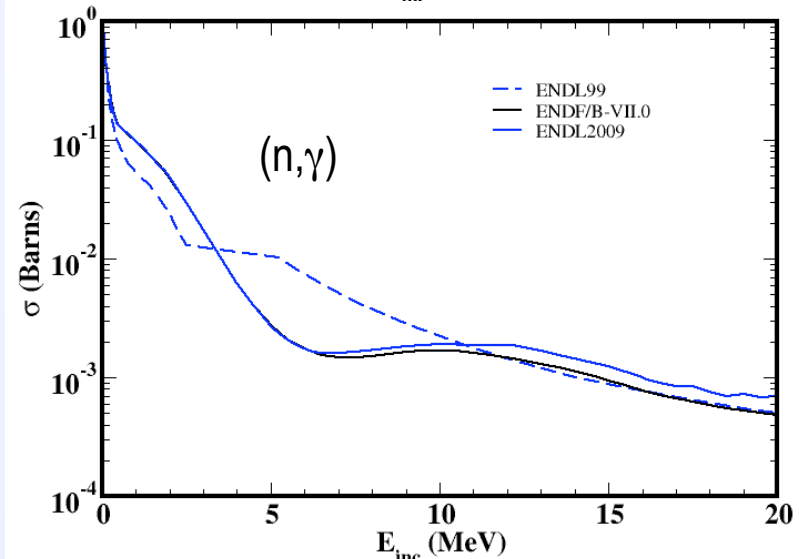
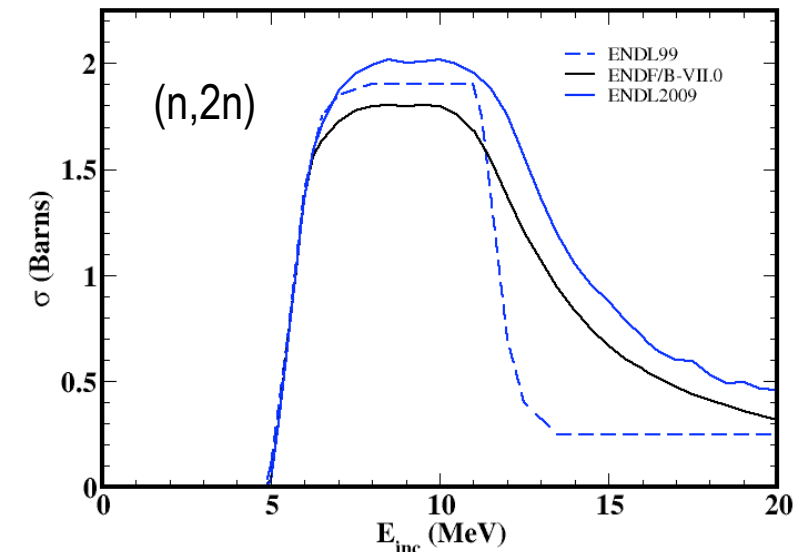
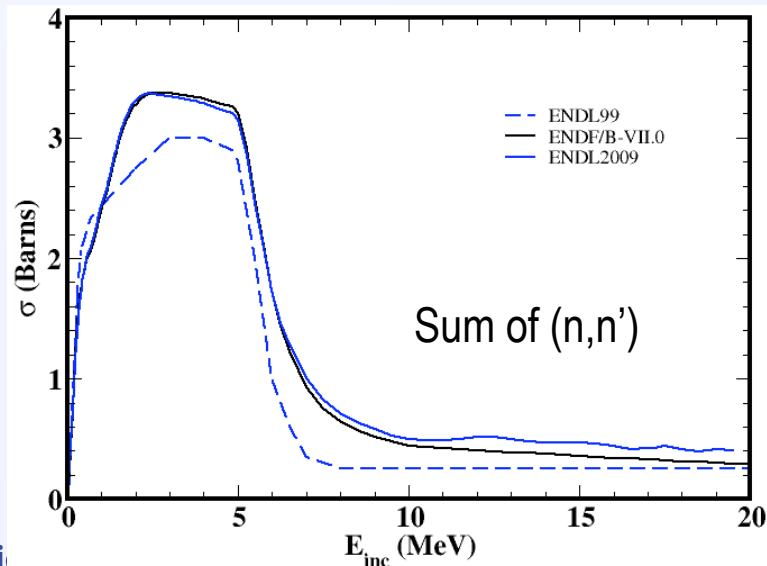
Fit folds in uncertainties from three classes of surrogate measurements: (t, pf), (^3He , xf) and (^{18}O , ^{17}O)

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:

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

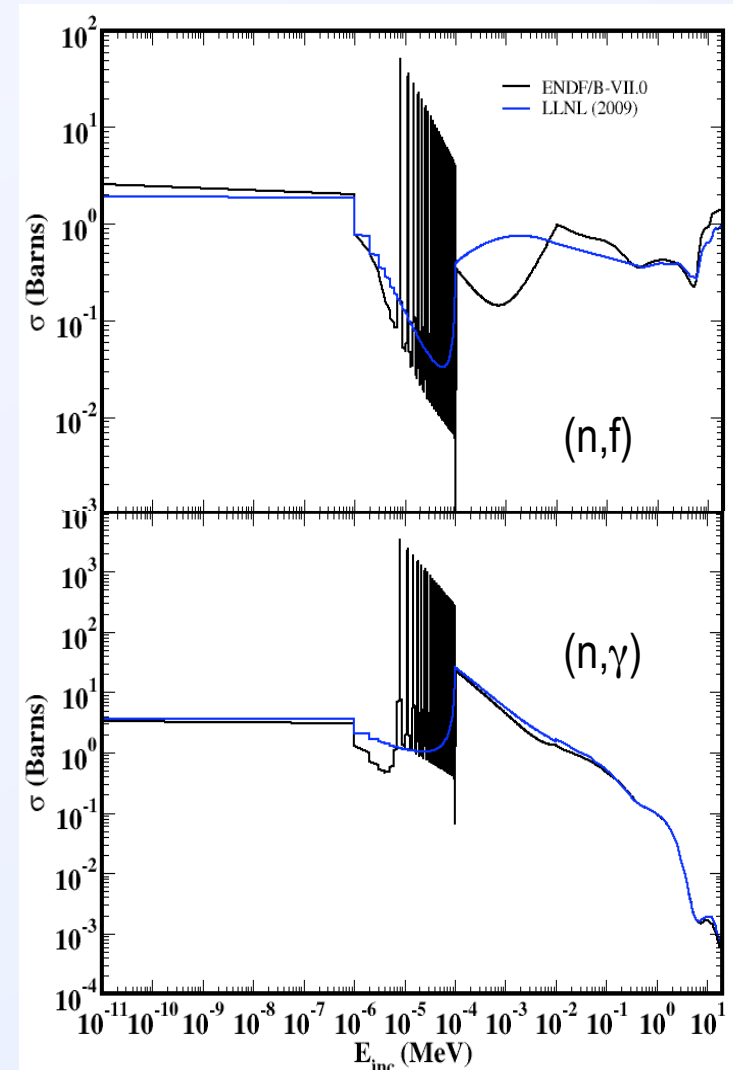


The original ^{239}U resonances required several fixes since they were a copy of the ^{237}U resonances

- 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
 - ^{57}Fe
 - ^{59}Co
 - Ni
 - Ta
 - Re
 - Pb
 - W
- Other Misc. evaluations

Light structural materials (FY08 Attribution L2 Milestone)

56 Ga	57 Ga	58 Ga	59 Ga	60 Ga	61 Ga	62 Ga	63 Ga	64 Ga	65 Ga	66 Ga	67 Ga	68 Ga	69 Ga	70 Ga	71 Ga	72 Ga	73 Ga	74 Ga
55 Zn	56 Zn	57 Zn	58 Zn	59 Zn	60 Zn	61 Zn	62 Zn	63 Zn	64 Zn	65 Zn	66 Zn	67 Zn	68 Zn	69 Zn	70 Zn	71 Zn	72 Zn	73 Zn
54 Cu	55 Cu	56 Cu	57 Cu	58 Cu	59 Cu	60 Cu	61 Cu	62 Cu	63 Cu	64 Cu	65 Cu	66 Cu	67 Cu	68 Cu	69 Cu	70 Cu	71 Cu	72 Cu
53 Ni	54 Ni	55 Ni	56 Ni	57 Ni	58 Ni	59 Ni	60 Ni	61 Ni	62 Ni	63 Ni	64 Ni	65 Ni	66 Ni	67 Ni	68 Ni	69 Ni	70 Ni	71 Ni
52 Co	53 Co	54 Co	55 Co	56 Co	57 Co	58 Co	59 Co	60 Co	61 Co	62 Co	63 Co	64 Co	65 Co	66 Co	67 Co	68 Co	69 Co	70 Co
51 Fe	52 Fe	53 Fe	54 Fe	55 Fe	56 Fe	57 Fe	58 Fe	59 Fe	60 Fe	61 Fe	62 Fe	63 Fe	64 Fe	65 Fe	66 Fe	67 Fe	68 Fe	69 Fe
50 Mn	51 Mn	52 Mn	53 Mn	54 Mn	55 Mn	56 Mn	57 Mn	58 Mn	59 Mn	60 Mn	61 Mn	62 Mn	63 Mn	64 Mn	65 Mn	66 Mn	67 Mn	68 Mn



Ian Thompson
(Attrib. structs.)



Neil Summers
(USNDP POC,
tool devel.)



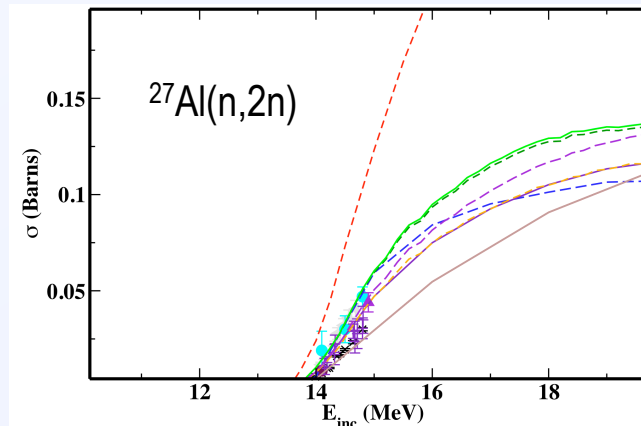
Rob Hoffman
(systematics, RadChem)

- 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)

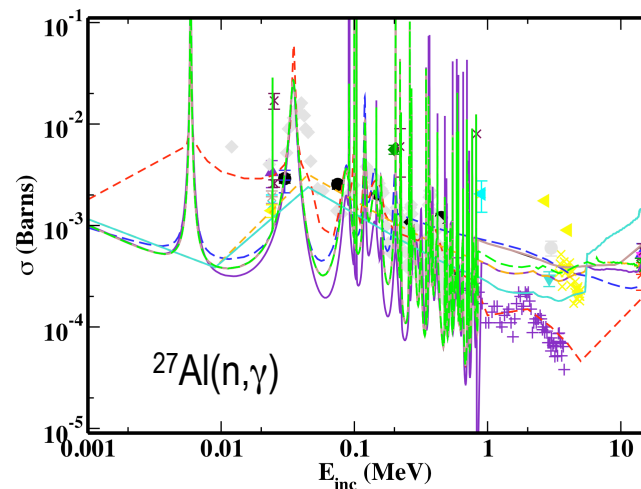
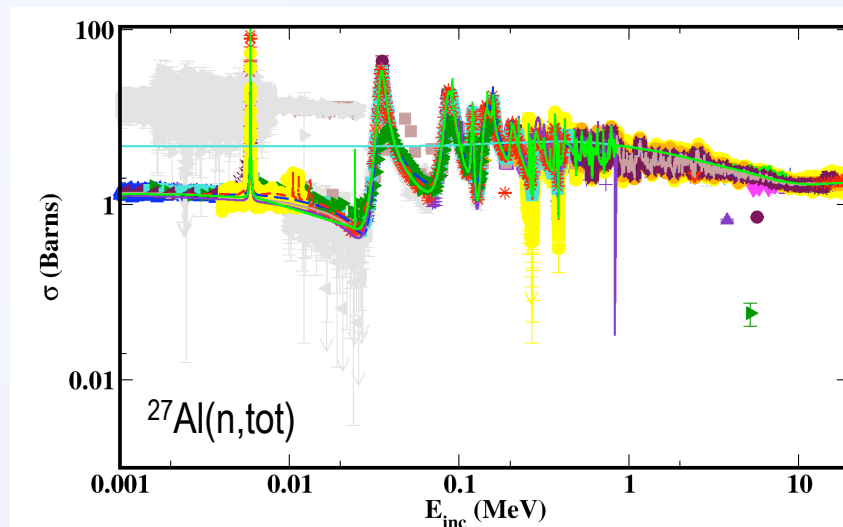
²⁵ Al	²⁶ Al	²⁷ Al	²⁸ Al	²⁹ Al
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- Stable ²⁷Al, want ²⁵⁻²⁹Al
- ²⁷Al: Resonance parameters defined up to 1 MeV, but still slight fluctuations up to 10 MeV.
- Resonances (to 1 MeV) from ENDF/B.VII
- Large (n,γ) data disagreements above 1 MeV!
- Large (n,tot) 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



Evaluations

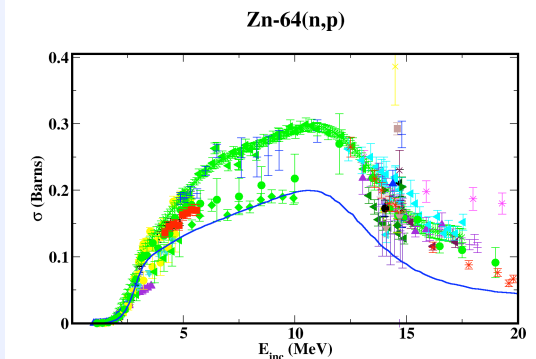
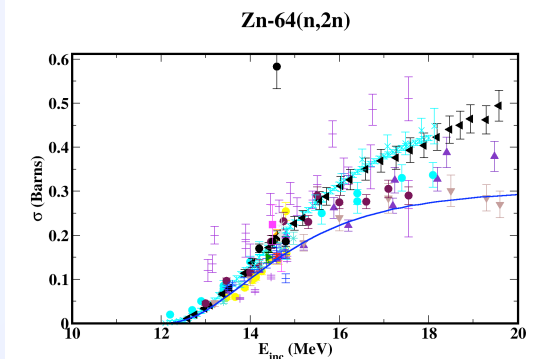
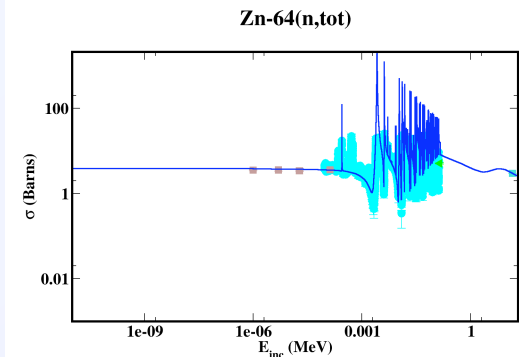
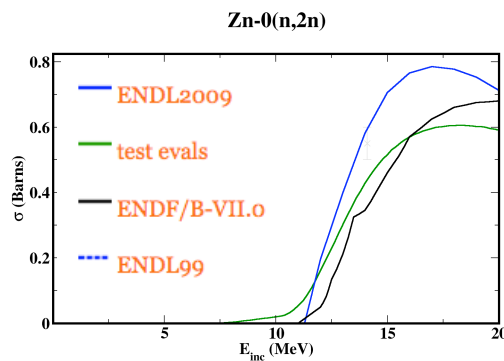
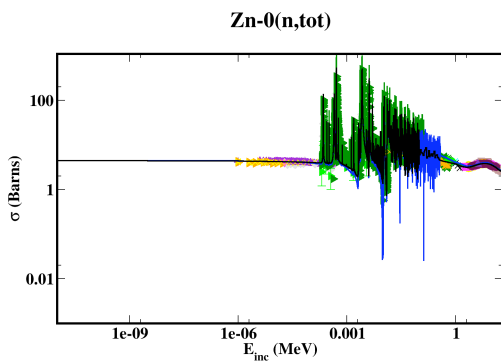
- endf.b-vii
- JEFF-3.1.1
- - JENDL-3.3
- ENDL2008
- TENDL2008
- - TALYS default
- New2009



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)

¹⁸⁶ Pb	¹⁸⁷ Pb	¹⁸⁸ Pb	¹⁸⁹ Pb	¹⁹⁰ Pb	¹⁹¹ Pb	¹⁹² Pb	¹⁹³ Pb	¹⁹⁴ Pb	¹⁹⁵ Pb	¹⁹⁶ Pb	¹⁹⁷ Pb	¹⁹⁸ Pb	¹⁹⁹ Pb	²⁰⁰ Pb	²⁰¹ Pb	²⁰² Pb	²⁰³ Pb	²⁰⁴ Pb	²⁰⁵ Pb	²⁰⁶ Pb	²⁰⁷ Pb	²⁰⁸ Pb	²⁰⁹ Pb	²¹⁰ Pb
¹⁸⁵ Tl	¹⁸⁶ Tl	¹⁸⁷ Tl	¹⁸⁸ Tl	¹⁸⁹ Tl	¹⁹⁰ Tl	¹⁹¹ Tl	¹⁹² Tl	¹⁹³ Tl	¹⁹⁴ Tl	¹⁹⁵ Tl	¹⁹⁶ Tl	¹⁹⁷ Tl	¹⁹⁸ Tl	¹⁹⁹ Tl	²⁰⁰ Tl	²⁰¹ Tl	²⁰² Tl	²⁰³ Tl	²⁰⁴ Tl	²⁰⁵ Tl	²⁰⁶ Tl	²⁰⁷ Tl	²⁰⁸ Tl	²⁰⁹ Tl
¹⁸⁴ Hg	¹⁸⁵ Hg	¹⁸⁶ Hg	¹⁸⁷ Hg	¹⁸⁸ Hg	¹⁸⁹ Hg	¹⁹⁰ Hg	¹⁹¹ Hg	¹⁹² Hg	¹⁹³ Hg	¹⁹⁴ Hg	¹⁹⁵ Hg	¹⁹⁶ Hg	¹⁹⁷ Hg	¹⁹⁸ Hg	¹⁹⁹ Hg	²⁰⁰ Hg	²⁰¹ Hg	²⁰² Hg	²⁰³ Hg	²⁰⁴ Hg	²⁰⁵ Hg	²⁰⁶ Hg	²⁰⁷ Hg	²⁰⁸ Hg
¹⁸³ Au	¹⁸⁴ Au	¹⁸⁵ Au	¹⁸⁶ Au	¹⁸⁷ Au	¹⁸⁸ Au	¹⁸⁹ Au	¹⁹⁰ Au	¹⁹¹ Au	¹⁹² Au	¹⁹³ Au	¹⁹⁴ Au	¹⁹⁵ Au	¹⁹⁶ Au	¹⁹⁷ Au	¹⁹⁸ Au	¹⁹⁹ Au	²⁰⁰ Au	²⁰¹ Au	²⁰² Au	²⁰³ Au	²⁰⁴ Au	²⁰⁵ Au		
¹⁸² Pt	¹⁸³ Pt	¹⁸⁴ Pt	¹⁸⁵ Pt	¹⁸⁶ Pt	¹⁸⁷ Pt	¹⁸⁸ Pt	¹⁸⁹ Pt	¹⁹⁰ Pt	¹⁹¹ Pt	¹⁹² Pt	¹⁹³ Pt	¹⁹⁴ Pt	¹⁹⁵ Pt	¹⁹⁶ Pt	¹⁹⁷ Pt	¹⁹⁸ Pt	¹⁹⁹ Pt	²⁰⁰ Pt	²⁰¹ Pt	²⁰² Pt				
¹⁸¹ Ir	¹⁸² Ir	¹⁸³ Ir	¹⁸⁴ Ir	¹⁸⁵ Ir	¹⁸⁶ Ir	¹⁸⁷ Ir	¹⁸⁸ Ir	¹⁸⁹ Ir	¹⁹⁰ Ir	¹⁹¹ Ir	¹⁹² Ir	¹⁹³ Ir	¹⁹⁴ Ir	¹⁹⁵ Ir	¹⁹⁶ Ir	¹⁹⁷ Ir	¹⁹⁸ Ir	¹⁹⁹ Ir						
¹⁸⁰ Os	¹⁸¹ Os	¹⁸² Os	¹⁸³ Os	¹⁸⁴ Os	¹⁸⁵ Os	¹⁸⁶ Os	¹⁸⁷ Os	¹⁸⁸ Os	¹⁸⁹ Os	¹⁹⁰ Os	¹⁹¹ Os	¹⁹² Os	¹⁹³ Os	¹⁹⁴ Os	¹⁹⁵ Os	¹⁹⁶ Os								
¹⁷⁹ Re	¹⁸⁰ Re	¹⁸¹ Re	¹⁸² Re	¹⁸³ Re	¹⁸⁴ Re	¹⁸⁵ Re	¹⁸⁶ Re	¹⁸⁷ Re	¹⁸⁸ Re	¹⁸⁹ Re	¹⁹⁰ Re	¹⁹¹ Re	¹⁹² Re	¹⁹³ Re										
¹⁷⁸ W	¹⁷⁹ W	¹⁸⁰ W	¹⁸¹ W	¹⁸² W	¹⁸³ W	¹⁸⁴ W	¹⁸⁵ W	¹⁸⁶ W	¹⁸⁷ W	¹⁸⁸ W	¹⁸⁹ W	¹⁹⁰ W	¹⁹¹ W	¹⁹² W										
¹⁷⁷ Ta	¹⁷⁸ Ta	¹⁷⁹ Ta	¹⁸⁰ Ta	¹⁸¹ Ta	¹⁸² Ta	¹⁸³ Ta	¹⁸⁴ Ta	¹⁸⁵ Ta	¹⁸⁶ Ta	¹⁸⁷ Ta	¹⁸⁸ Ta	¹⁸⁹ Ta	¹⁹⁰ Ta											

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.



Ian Thompson
(Attrib. structs.)



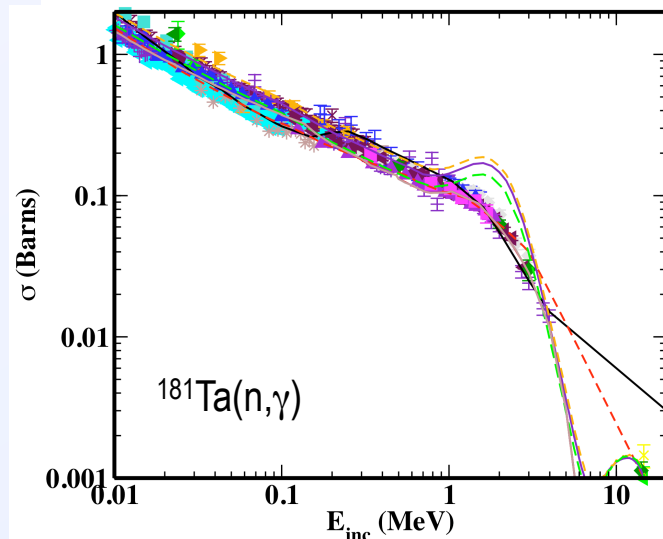
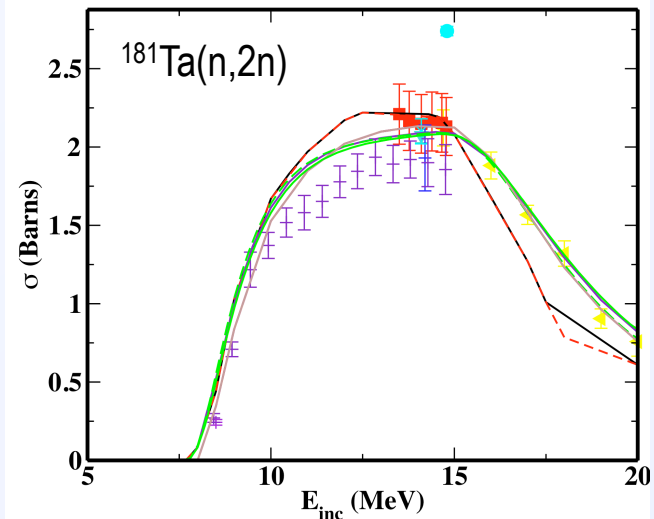
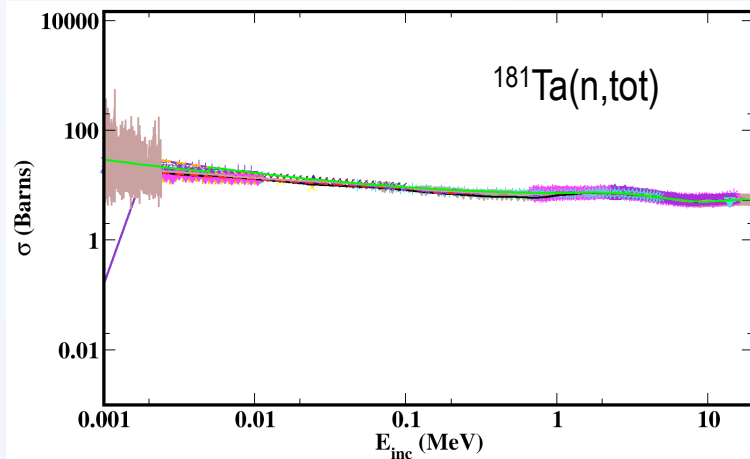
Neil Summers
(USNDP POC,
tool devel.)



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

Ta (Z=73)

- Only ^{181}Ta is stable, want $^{178-183}\text{Ta}$.
- (^{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

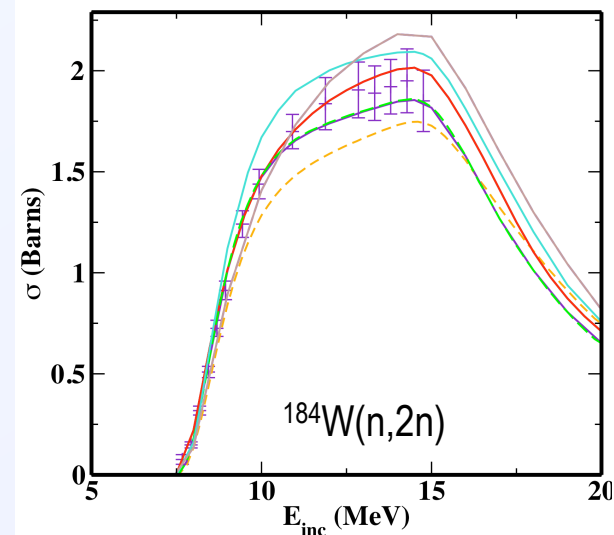
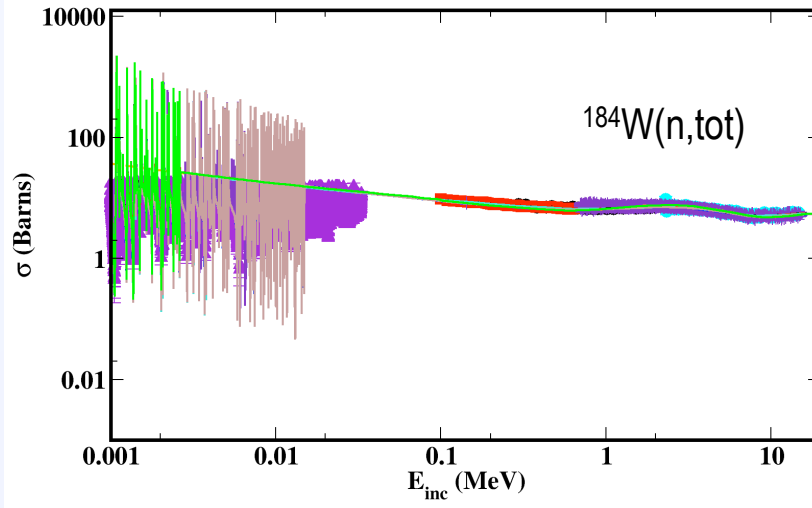


Evaluations

- endf.b-vii
- JEFF-3.1.1
- - - JENDL-3.3
- ENDL2008
- TENDL2008
- - - TALYS default
- New2009

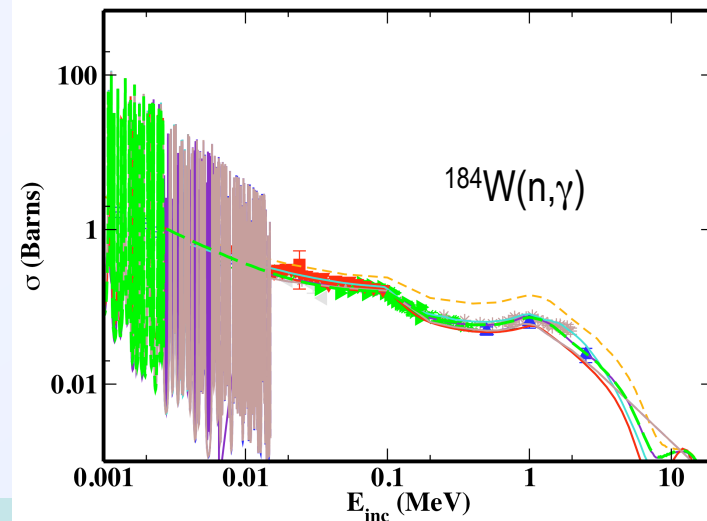
W (Z=74)

- Stable $^{180,182-4,186}\text{W}$, want also $^{178-9,181,185,187-8}\text{W}$.
- 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



Evaluations

- endf.b-vii
- JEFF-3.1.1
- JENDL-3.3
- ENDL2008
- TENDL2008
- TALYS default
- New2009
- IAEA

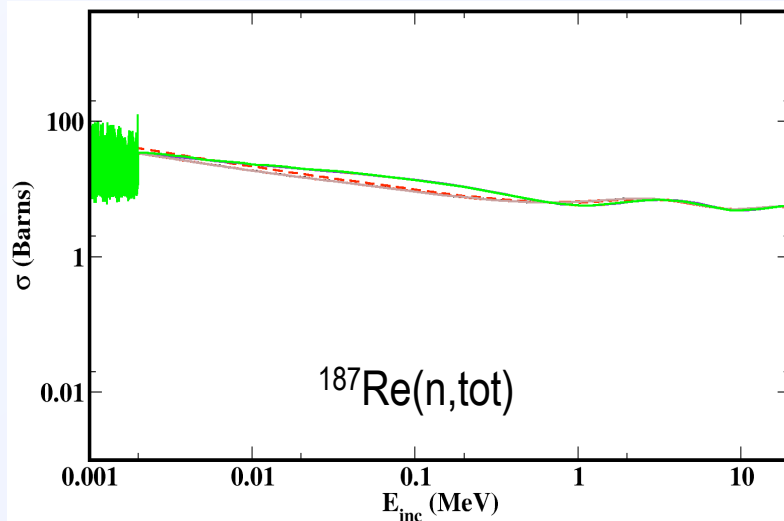


We are submitting the unstables to ENDF/A for

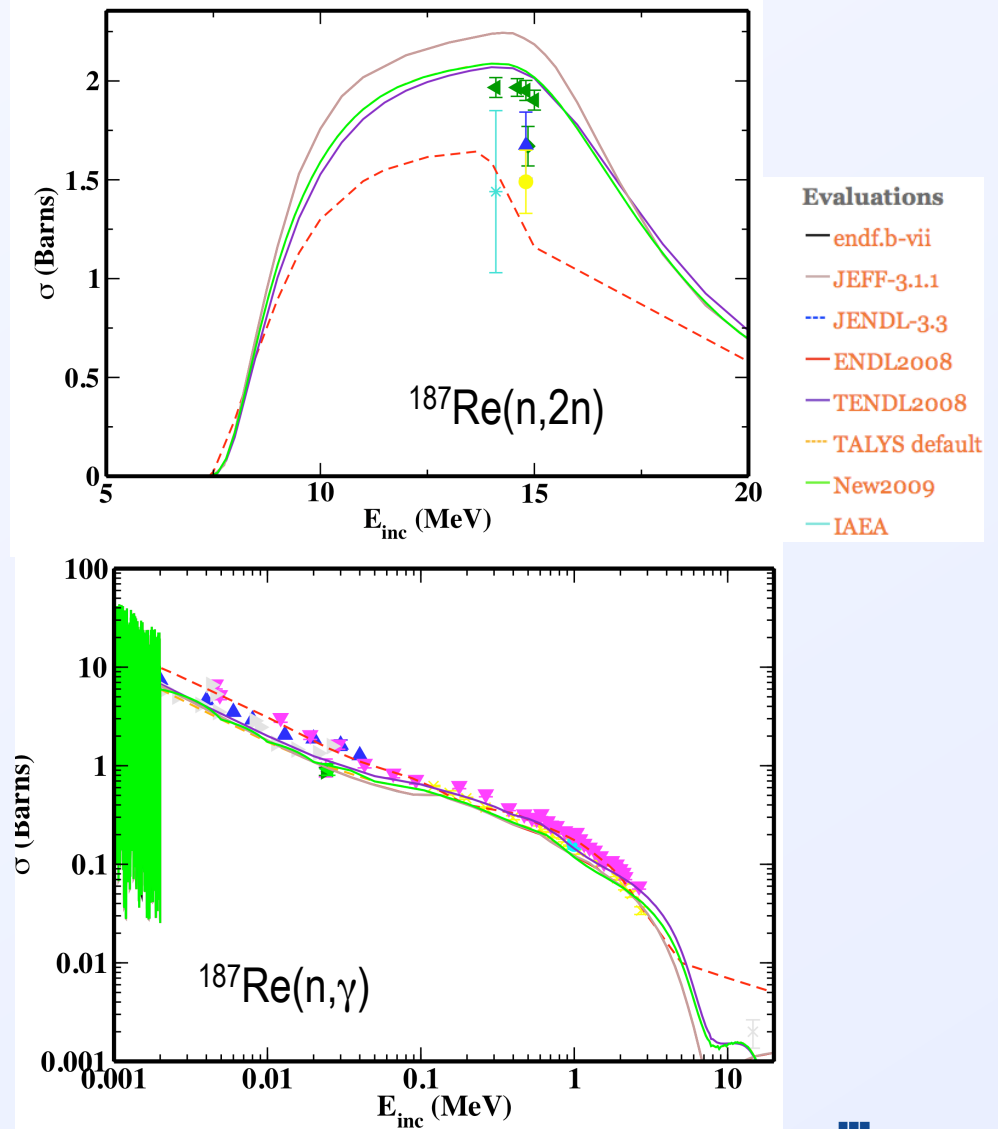
(we hope) inclusion in ENDF/B-VII.1, we recommend the IAEA W evals for the stables

Re (Z=75)

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



We are submitting these 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

- 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)



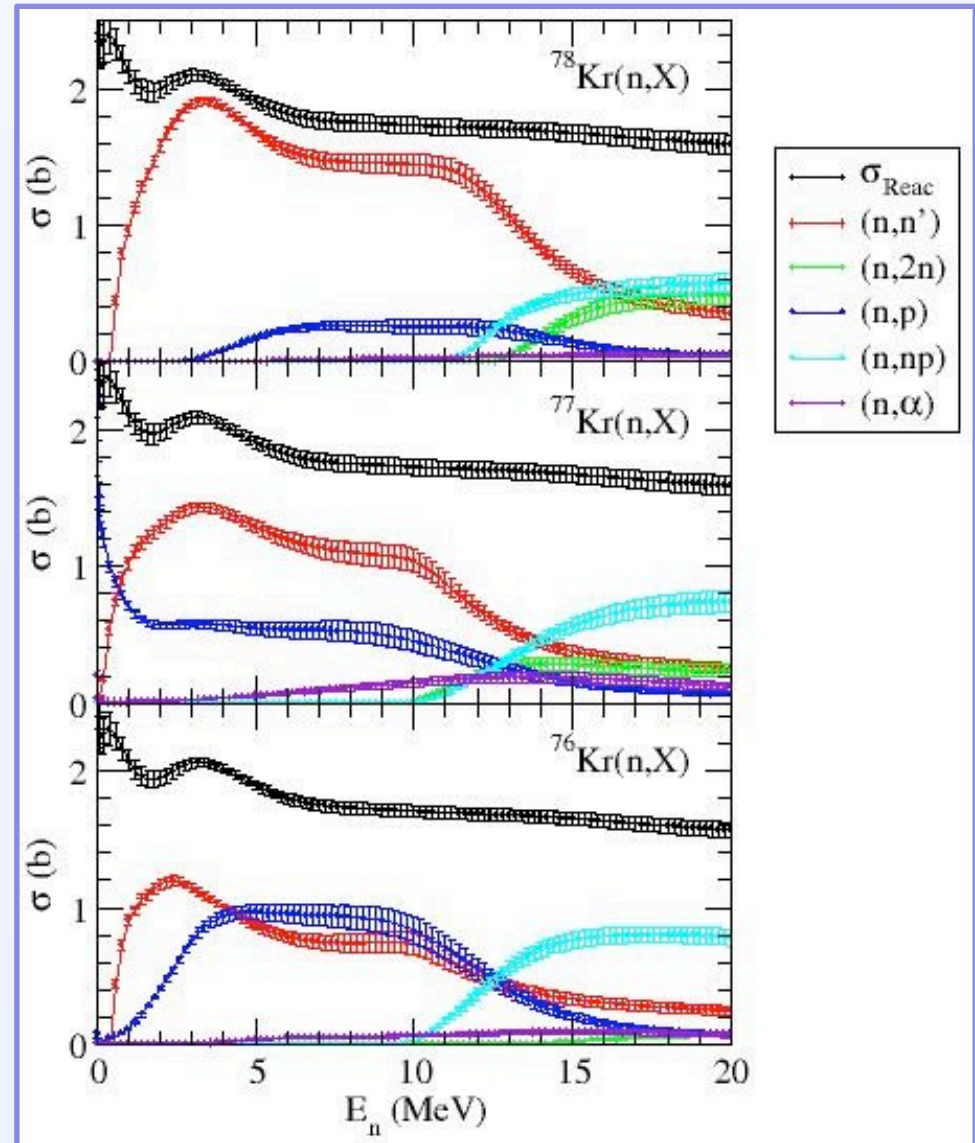
Neil Summers
(USNDP POC,
tool devel.)

Kr isotopes

⁷⁶ Kr	⁷⁷ Kr	⁷⁸ Kr	⁷⁹ Kr	⁸⁰ Kr	⁸¹ Kr	⁸² Kr	⁸³ Kr	⁸⁴ Kr	⁸⁵ Kr	⁸⁶ Kr
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- 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

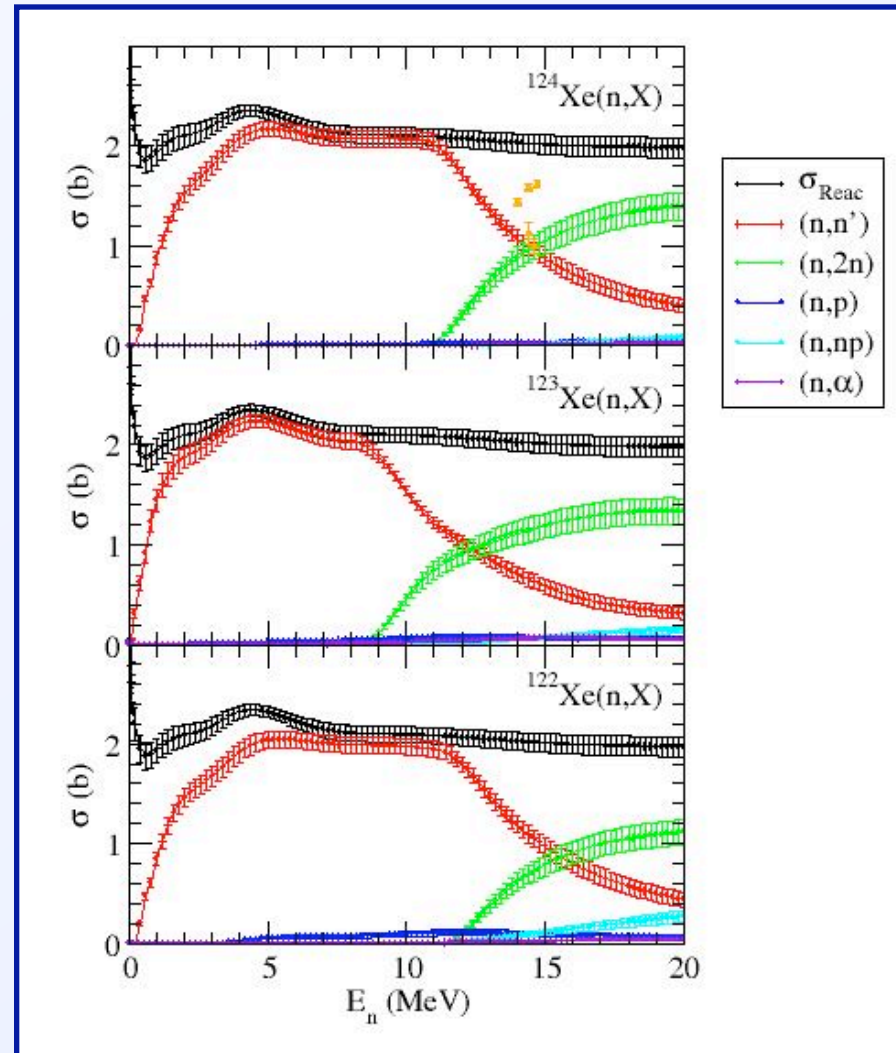


Xe isotopes

¹²² Xe	¹²³ Xe	¹²⁴ Xe	¹²⁵ Xe	¹²⁶ Xe	¹²⁷ Xe	¹²⁸ Xe

- Small charge-particle channels, neutron channels are reliable

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

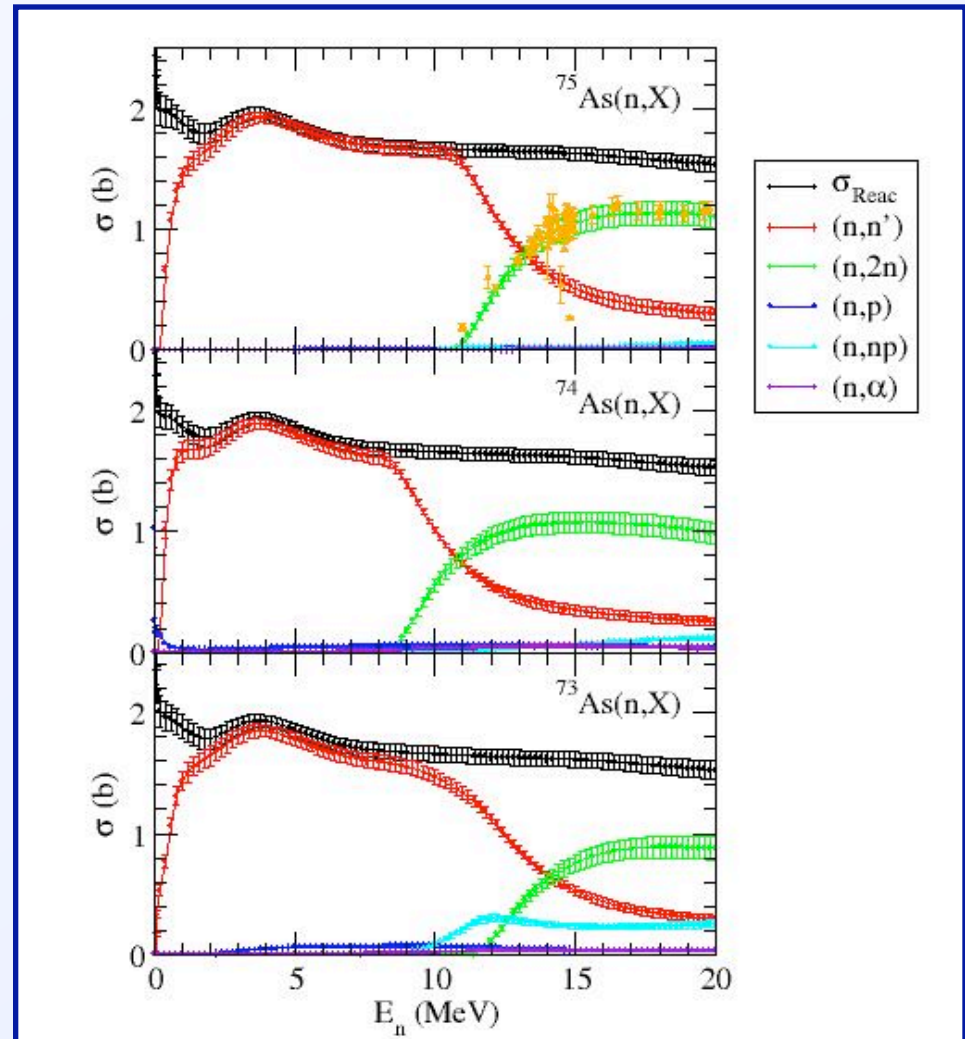


As isotopes

⁷³ As	⁷⁴ As	⁷⁵ As
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- 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 ^{240}Am resonances for ENDF/B-VII.1
 - ^{237}U needs review
 - ^{239}U submitted for ENDF/B-VII.1
- **Structural materials**
 - Not ready: Pb?, Zn, Co
 - Not worth submitting: ^{57}Fe
 - 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):

