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Nuclear Validation Efforts at Livermore

Computational Nuclear Physics

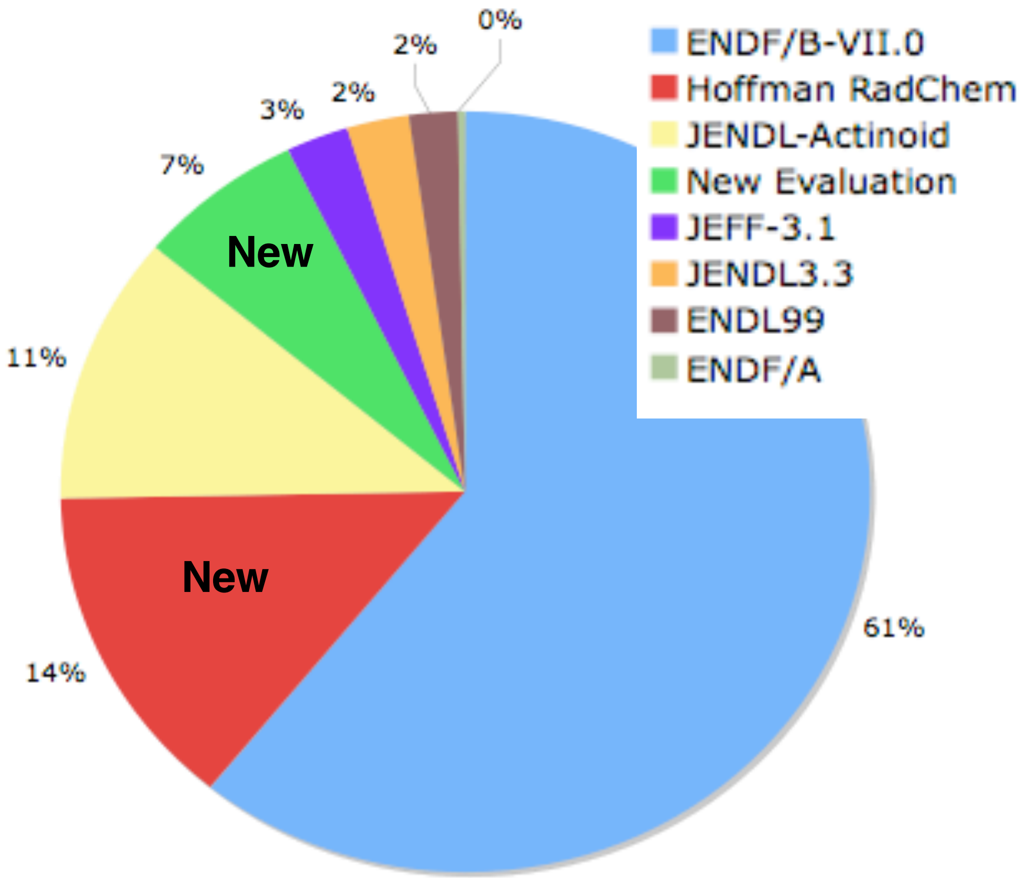
Marie-Anne Descalle, Dave Brown,

Jason Pruet

S&T - PhySci/N Division

Lawrence Livermore National Laboratory

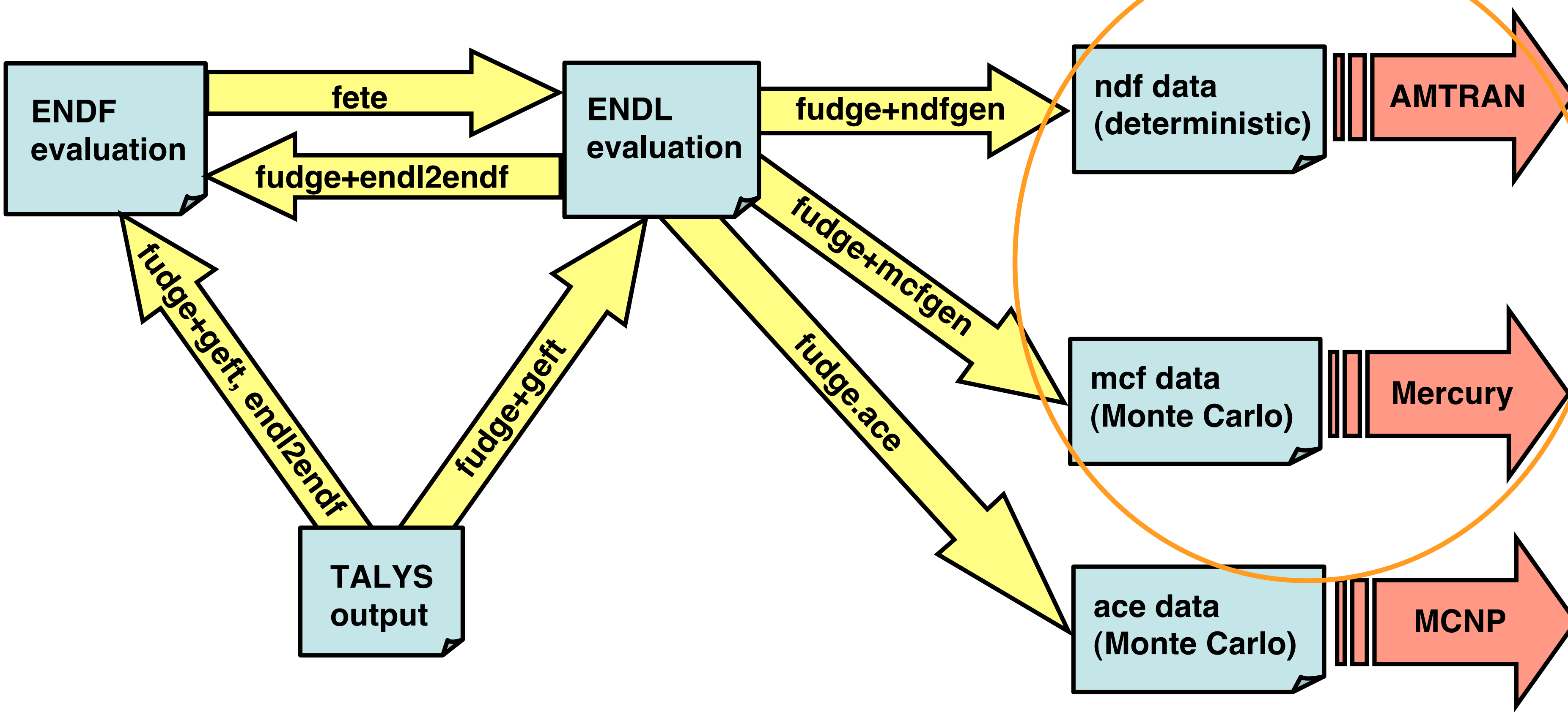
We have released the next major ENDL; 61% is translated from ENDF/B-VII.0



- ENDL2008 contains nearly 400 more isotopes than ENDL99, 79% are translated from external libraries.
- 21% is new (see Neil Summers' presentations)
- For the ENDL release, we focused on incident neutrons

Over the last few years we've built a validation basis for our data.

LLNL nuclear data processing system is complex, with many subsystems that require extensive testing



Our testing focuses on deterministic transport with AMTRAN and Monte Carlo transport with Mercury.

We have developed several simple tests to ensure that our libraries run

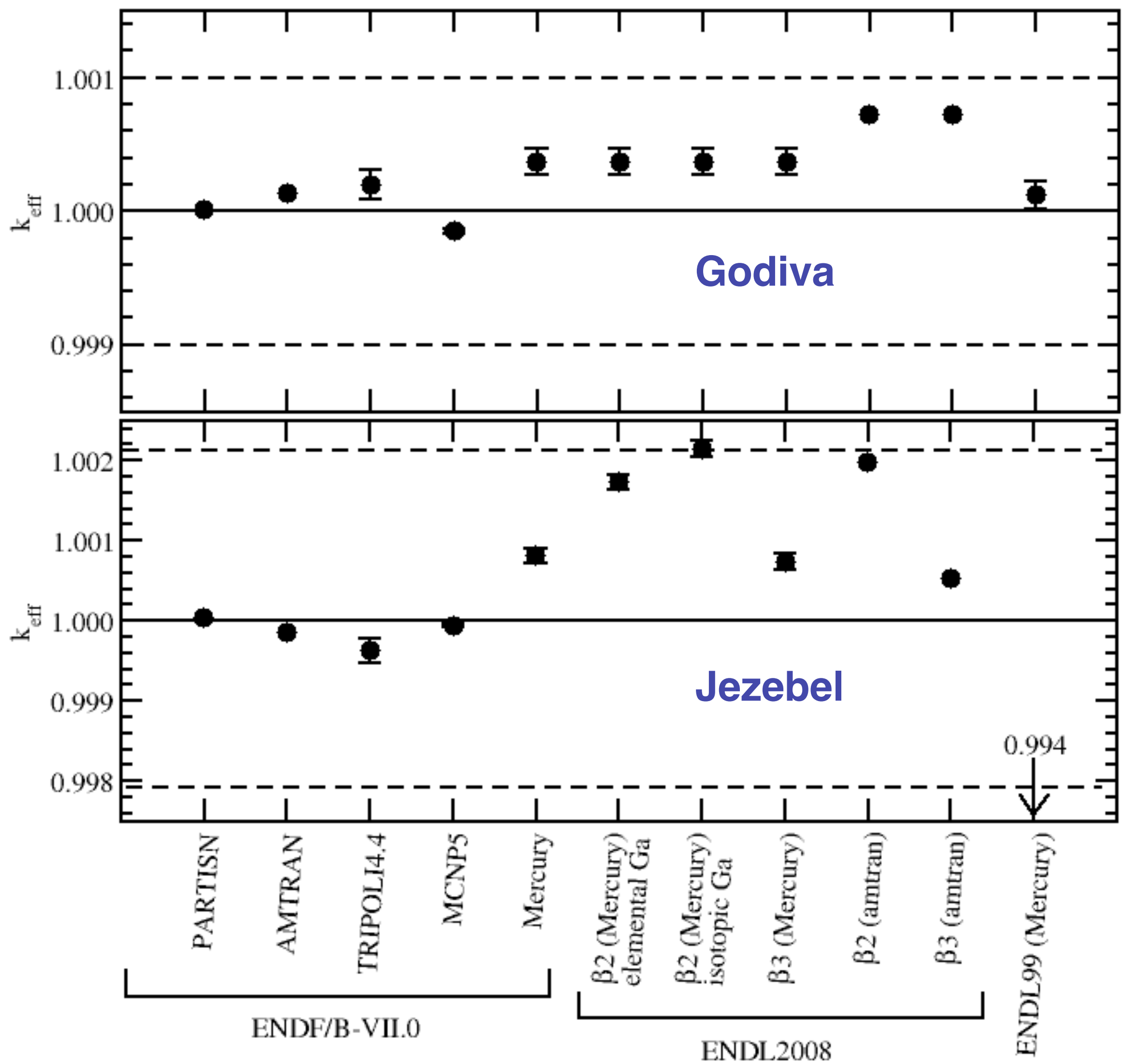
Simple sanity checks of processed data

- **MCF files using Mercury:**
  - Crash test: dynamic simulation of sphere of material with neutron source in middle
  - Gamma production test: count average γ energy leaked out per source neutron
- **NDF files using AMTRAN:**
  - k_{eff} calculation: ENDL99's ^{239}Pu as fuel, material of interest as reflector

(n,g) Loop **apr-3-08**

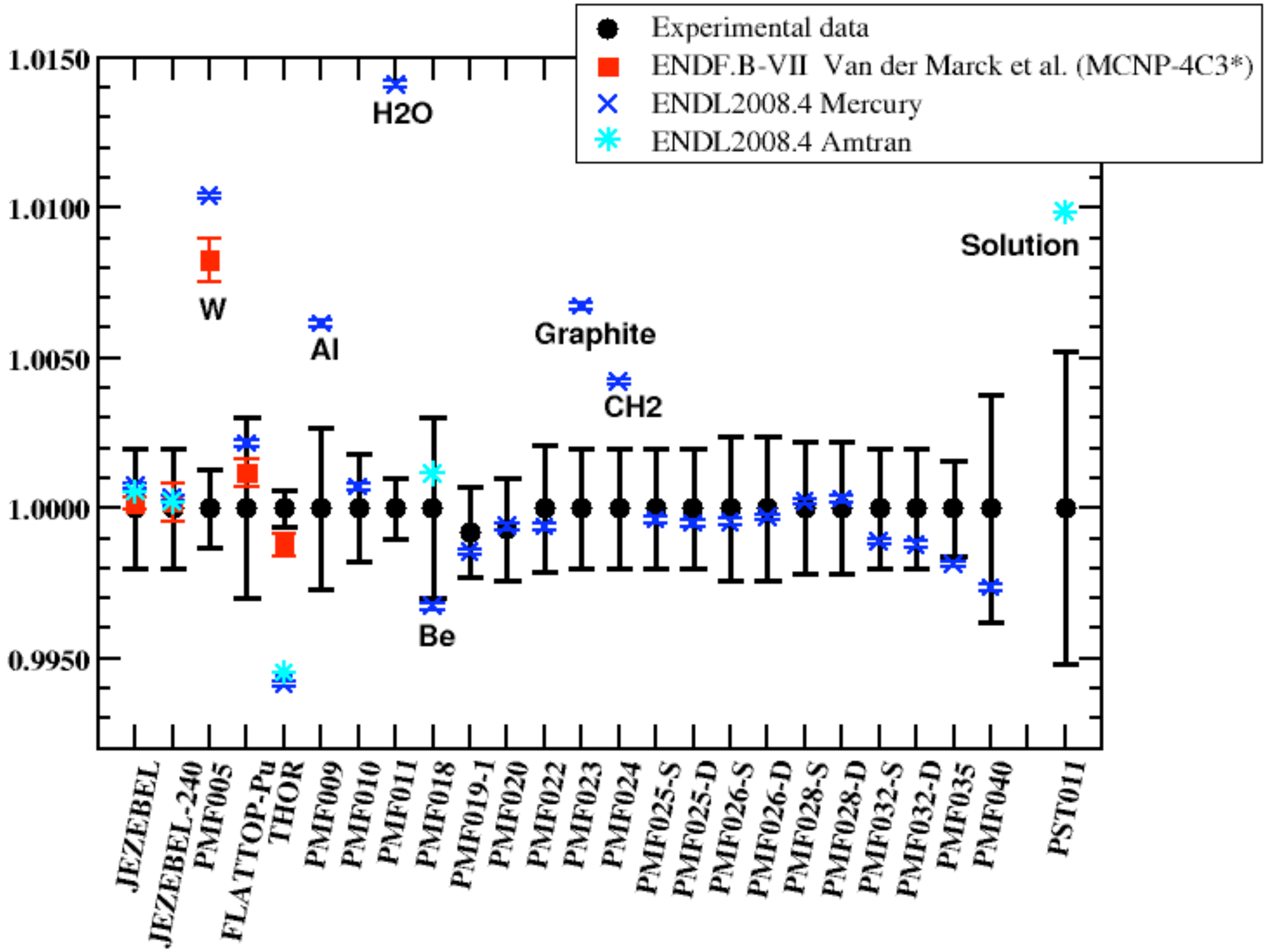
	endl2008.actinides (g MeV/n)	ENDFB-VII.0 (g MeV/n)	Difference endl/endf
za092232	1.30997	1.32221	0.9%
za092233	0.61724	0.62760	1.7%
za092234	0.68177	0.68190	0.0%
za092235	1.15799	1.18102	1.9%
za092236	0.48062	0.47381	-1.4%
za092237	0.41975	0.42931	2.2%
za092238	0.32453	0.32735	0.9%
za092239	0.35385	0.35976	1.6%
za092240	0.25568	0.24407	-4.8%
za092241	0.19885	0.19776	-0.5%
za093235	0.03820	0.03254	-17.4%
za093236	0.03295	0.02616	-25.9%
za093237	0.61327	0.60487	-1.4%
za093238	0.01676	0.01333	-25.7%
za093239	0.05851	0.05703	-2.6%
za094236	0.01509	0.01090	-38.4%
za094237	0.89765	0.01072	-8274.0%
za094238	0.01784	0.02923	39.0%
za094239	0.84728	0.81222	-4.3%
za094240	0.77121	1.33084	42.1%
za094241	0.02321	0.94248	97.5%
za094242	0.13308	1.10094	87.9%
za094243	0.61741	0.64375	4.1%
za094244	0.01492	0.00429	-247.8%
za094246	0.19694	0.18790	-4.8%

ENDL2008's performance is comparable to ENDF/B-VII.0 for bare assemblies

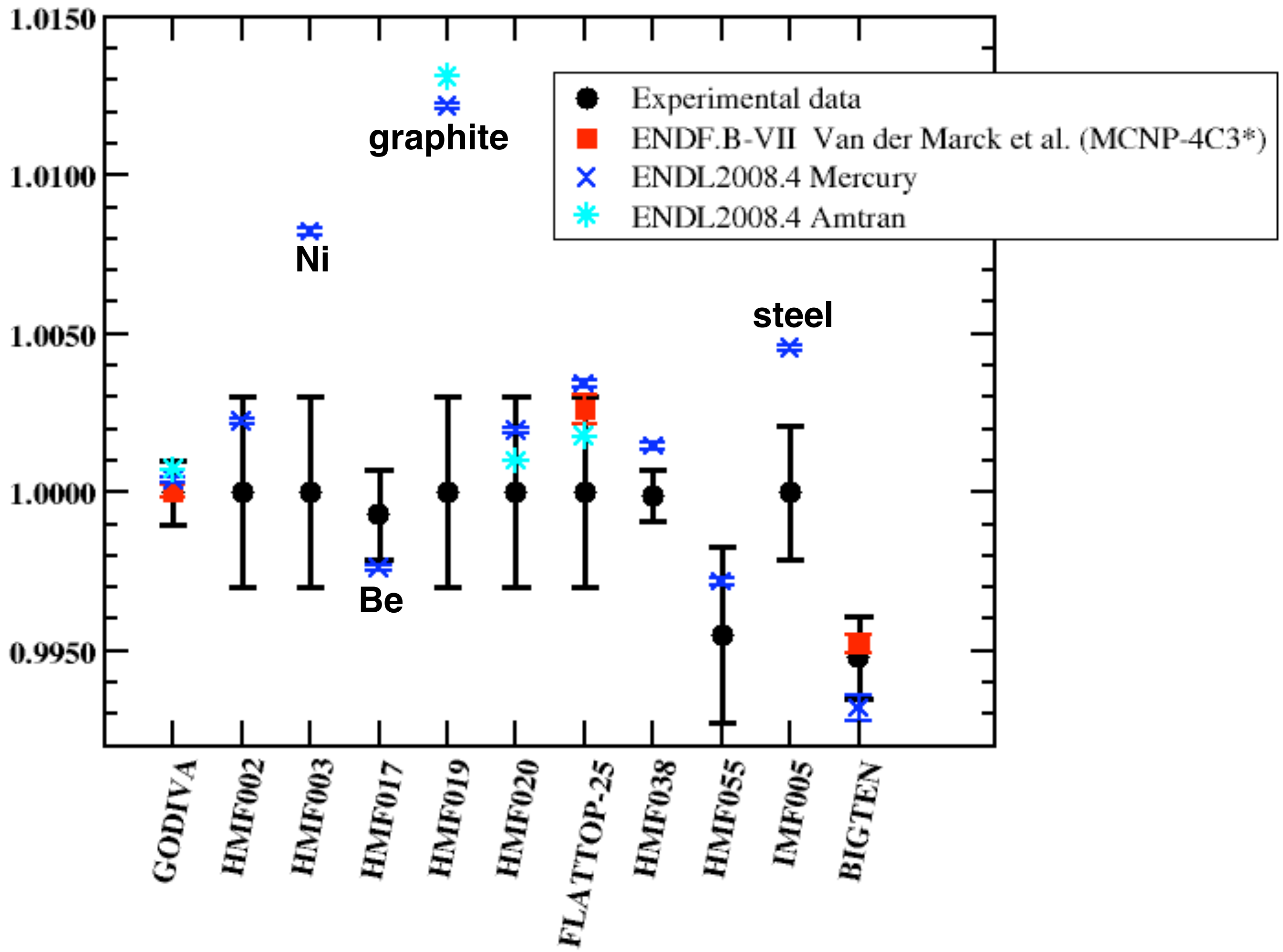


- Godiva k_{eff} in excellent agreement with ENDF/B-VII.0, even for ENDL99
- Jezebel k_{eff} has improved dramatically since ENDL99
- ENDL99's elemental Ga evaluation now replaced with new isotopic evaluations
- ^{240}Pu evaluation from JENDL-Actinoid library responsible for $\beta 2 \rightarrow \beta 3$ improvement

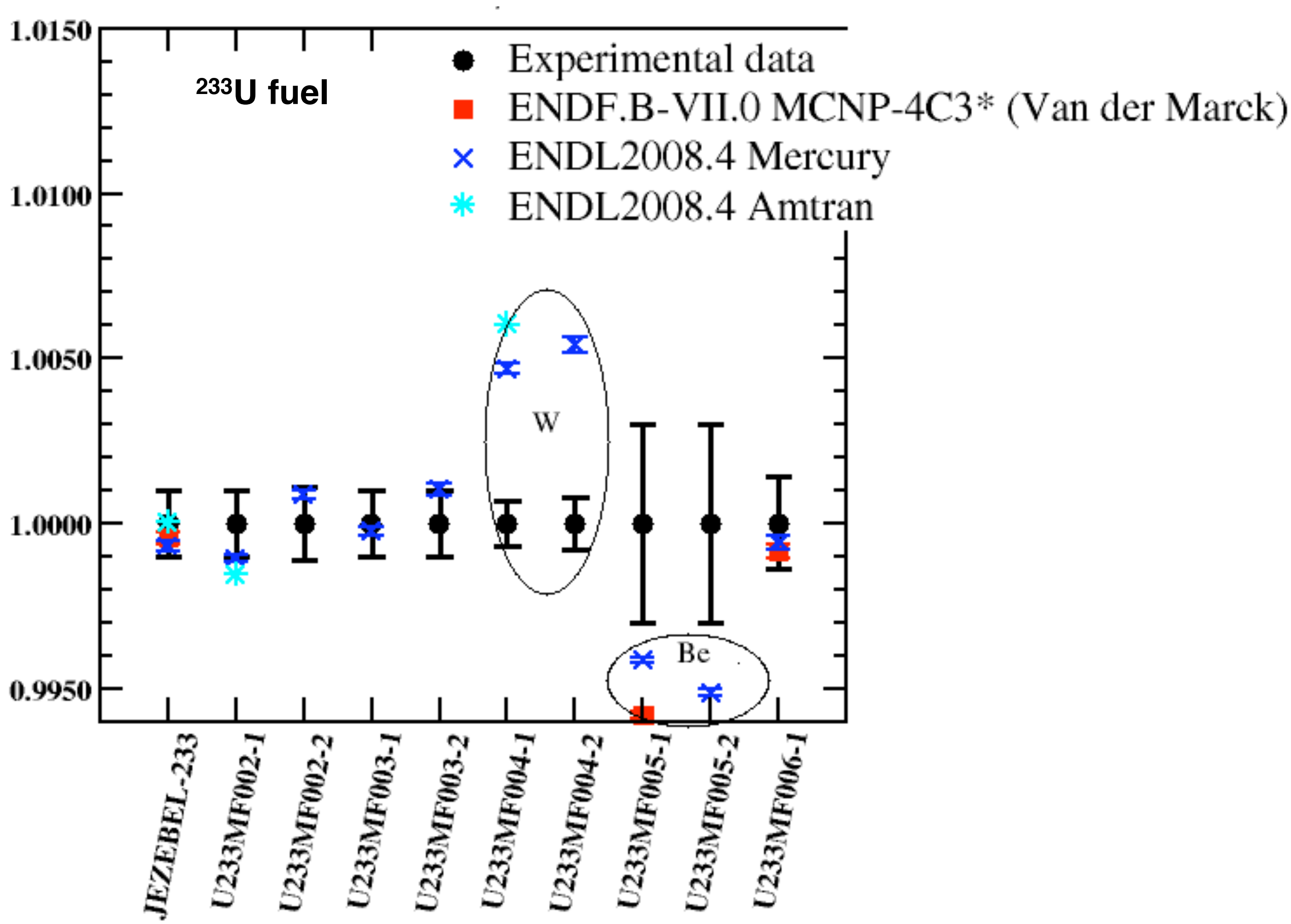
Criticality benchmarks
ENDL2008 performance in Pu assemblies



Criticality benchmarks
ENDL2008 performance in ^{235}U assemblies



Criticality benchmarks
ENDL2008 performance in ^{233}U assemblies



Criticality benchmarks
ENDL2008 & ENDF/B-VII.0 summary

- ENDL2008:
  - Poor $S_{\alpha\beta}$ support means poor performance for thermal assemblies (PST11, HMF19, PMF11, PMF23, PMF24)
  - URR treatment not in production code nor data library yet

- ENDL2008 & ENDF/B-VII.0
  - Ni problem for all libraries (HMF3)
  - W problem for all libraries (PMF5, U233MF4)
  - Be problem for all libraries (HMF17, PMF18)
  - Thor difference is an understood input deck problem

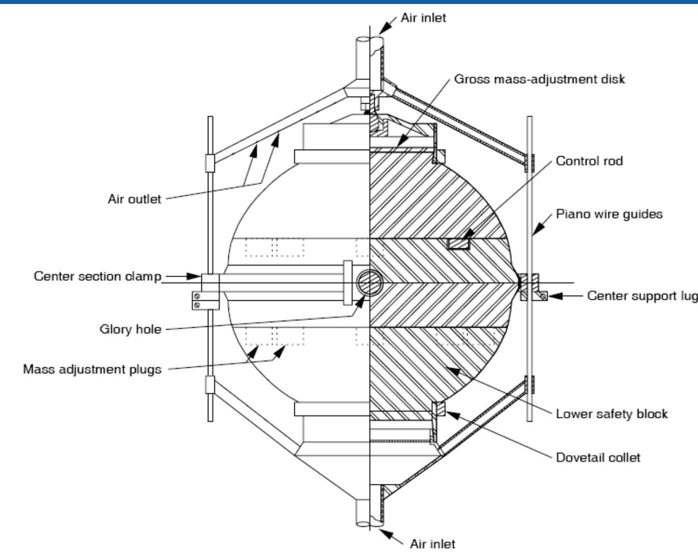
For some time we’ve been developing calculations of material worth for validation

- Test change in k_{eff} as move small slug of material radially
- Defined as the change in reactivity ($) per mole of material

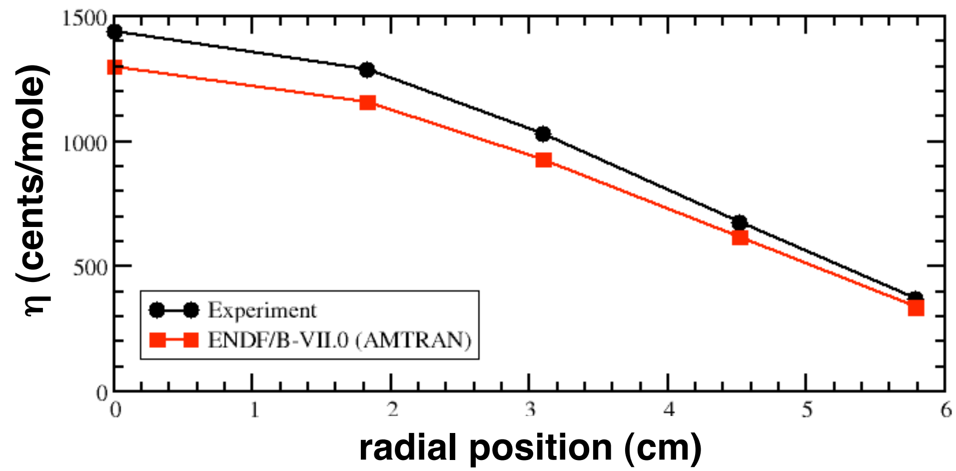
$$\eta = \frac{d\rho}{dm}$$

- In the center: replacement coefficient is sensitive to the absorption cross section
- At the outer surface: replacement coefficient is sensitive to the scattering cross section

Though the k-eigenvalues agree, results for worth are inconsistent (change β_{eff}?).



0.5” d. x 0.5” l. Pu slug in Jezebel:

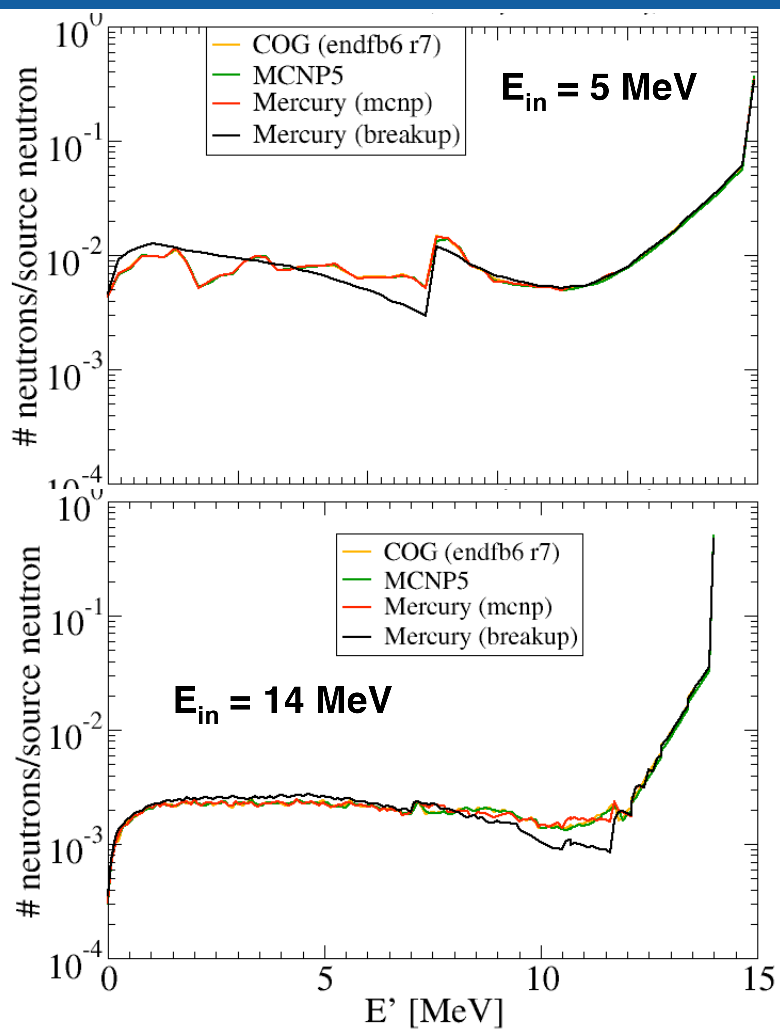


When translating ENDF/B-VII.0's ^{6}Li for inclusion in ENDL2008, we ran into a problem…

- **A bit of history:**
  - In the 1970's, one could not store $dN(E)/d\mu dE'$ data in ENDF
  - For ^{6}Li(n,nd)α (and other reactions) this is a problem…
  - Clever folks at LANL developed a work-around:
    - Create fake (n,n') "levels" w/ kinematics rigged to produce correct neutron distribution
    - Denote correct reaction with LR flag
    - Ignore all the other outgoing particles
  - Several evaluations use this format: ^{6}Li, ^{7}Li, ^{11}B, ^{nat}C, ^{14}N
- **Problems with this approach:**
  - Not all particles accounted for: ^{6}Li(n,nd)α called ^{6}Li(n,n')
  - Format use not documented

We have attempted to translate what the evaluator meant, rather than what's in the files: results need testing

We have developed simple pencil-beam on broomstick test to validate handling of break-up data

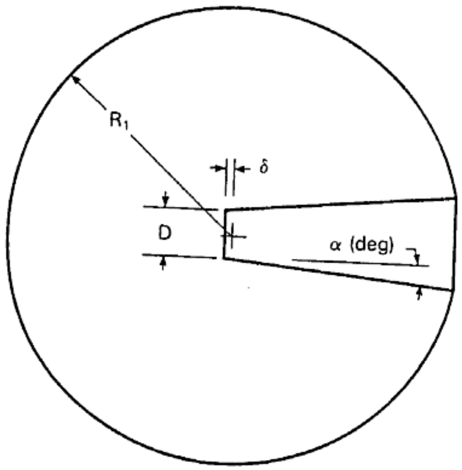


Energy [MeV]	Collision Event	ENDF.B-VIr7 COG	ENDL99	ENDF.B-VII.0 Mercury	ENDF.B-VI r2 Mercury
5	Elastic	407403	431020	404302	431827
	(n,n'g)	233380	2429	2331	1593
	(n,2n'ag)	2324	0	2410	2435
	(n,pg)	9158	6400	9054	9049
	(n,tg)	26744	26433	26355	26535
	(n,g)	3	15	2	2
	nd	**0**	**210937**	**235541**	**206182**
	total # coll.	*679012*	*677234*	*679995*	*677623*
14	Elastic	321520	353101	321283	361187
	(n,n'g)	177495	1201	546	1105
	(n,2n'ag)	28995	0	29139	29126
	(n,pg)	2175	2759	2302	29126
	(n,tg)	9548	12308	9718	9719
	(n,g)	6	8	5	5
	nd	**0**	**102305**	**177301**	**137114**
	total # coll.	*539739*	*471682*	*540294*	*567382*

- ^{6}Li, subtle differences in neutron distribution; more dramatic for ^{7}Li, ^{14}N
- # produced deuterons wildly different
- Difficult to trust validity of results w/o proper documentation of format

We recommend re-evaluating ^{6}Li, ^{7}Li, ^{11}B, ^{nat}C and ^{14}N

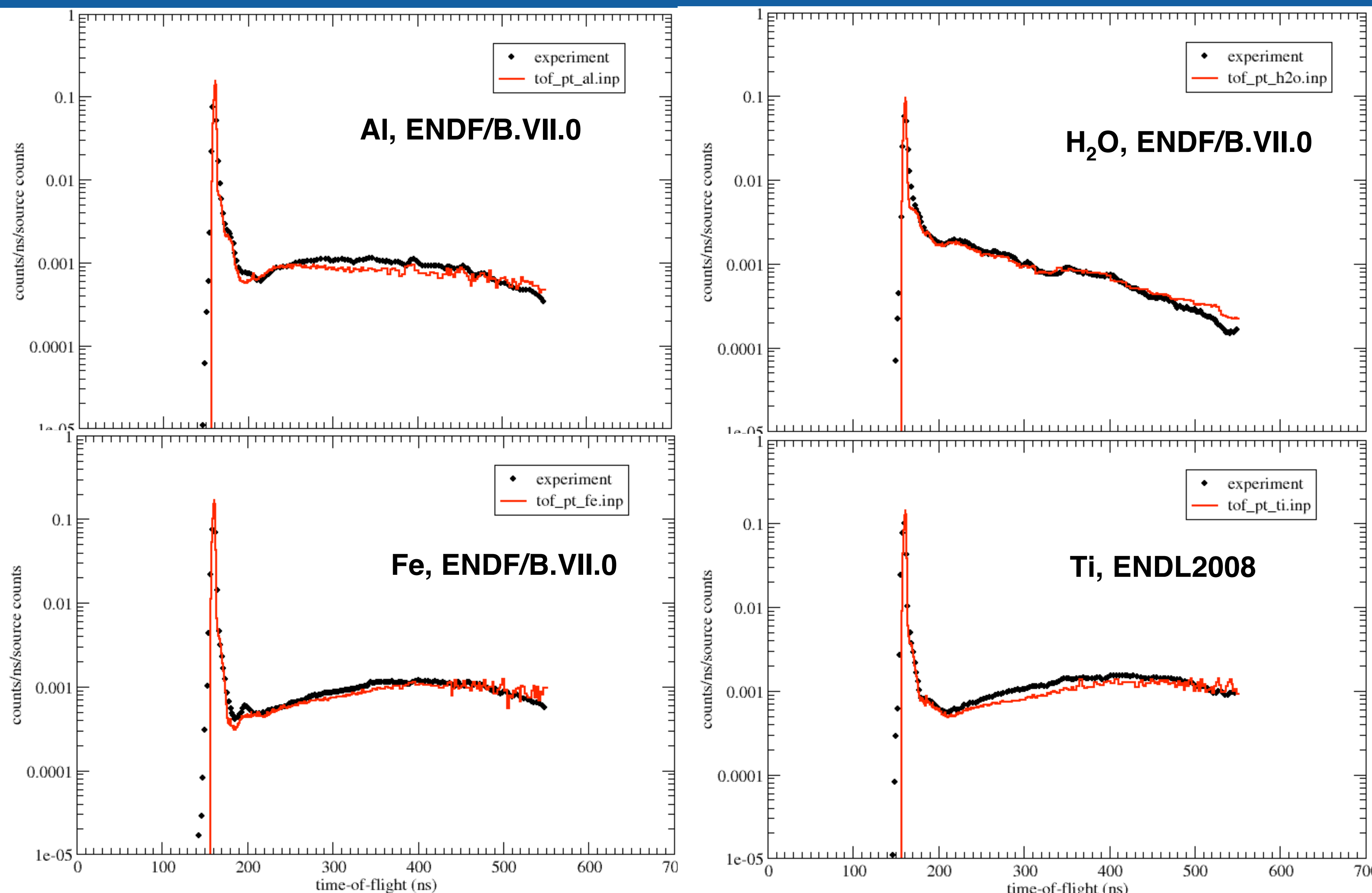
We have developed Mercury models of LLNL Pulsed sphere experiments published by Goldberg (1990)



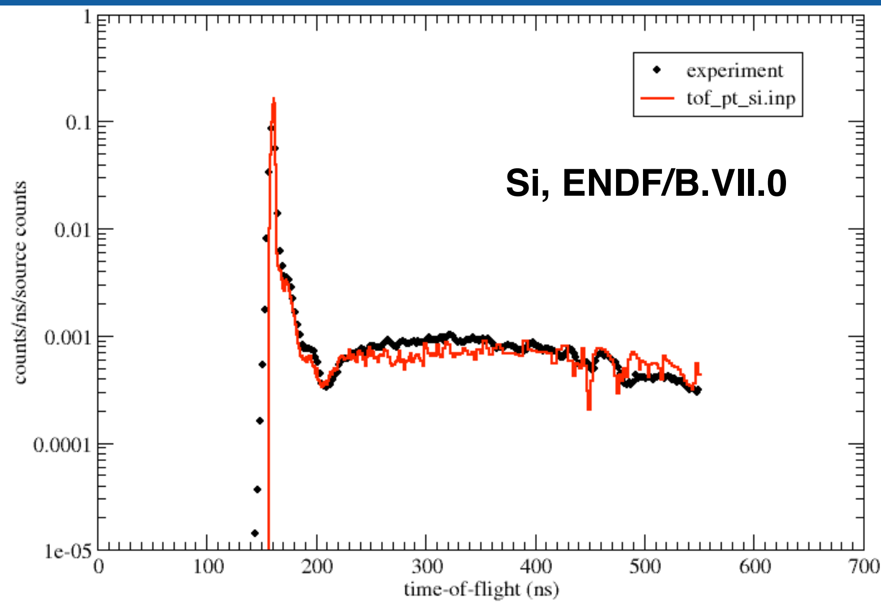
- LLNL Pulsed sphere program 1970's-80's
  - Pulsed 14 MeV neutrons; d-t source
  - Measure neutron and γ spectra (TOF)
- Model of experiment including detector efficiency, source correlation
- 17 different materials
  - ($25\ g/cm^2 < \rho R < 45 g/cm^2$)

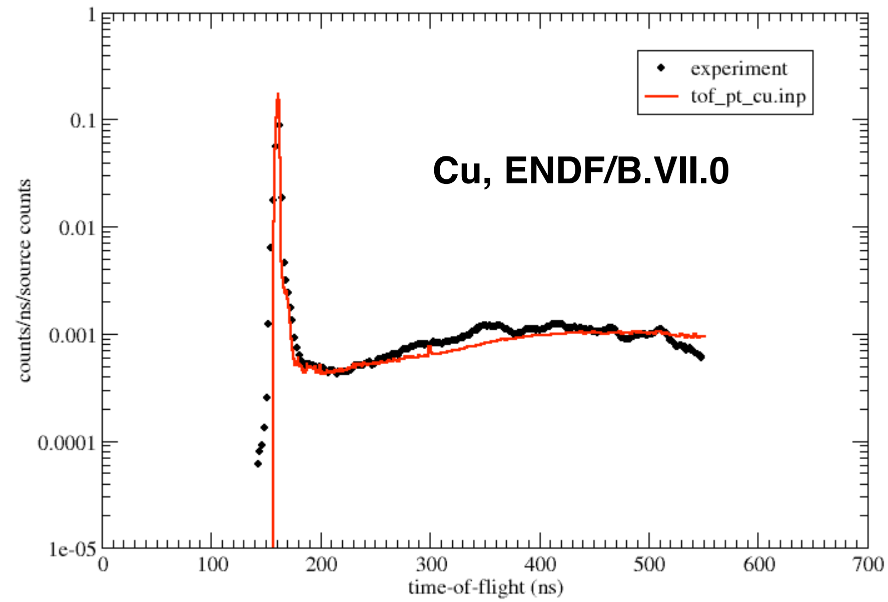
	ENDL2008 Source
H_2O	ENDF/B-VII.0
Al	ENDF/B-VII.0
Si	ENDF/B-VII.0
Fe	ENDF/B-VII.0
Cu	ENDF/B-VII.0
W	ENDF/B-VII.0
Au	ENDF/B-VII.0
Pb	ENDF/B-VII.0
^{232}Th	ENDF/B-VII.0
^{235}U	ENDF/B-VII.0
^{238}U	ENDF/B-VII.0
^{239}Pu	ENDF/B-VII.0
C_2F_4	ENDL99/ENDF/B-VII.0
C	ENDL99
N	ENDL99
Ti	JENDL-3.3
Ta	JEFF-3.1

H_20, Al, Fe and Ti are in fairly good agreement with experiments

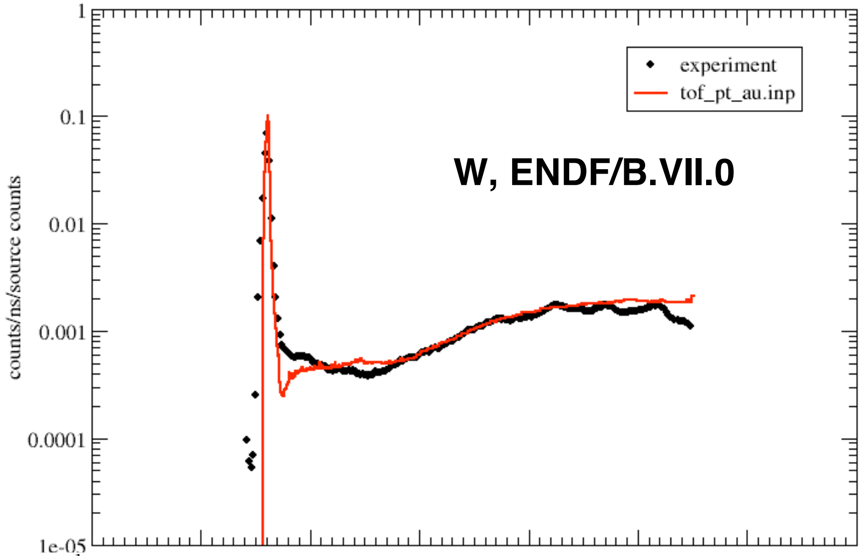


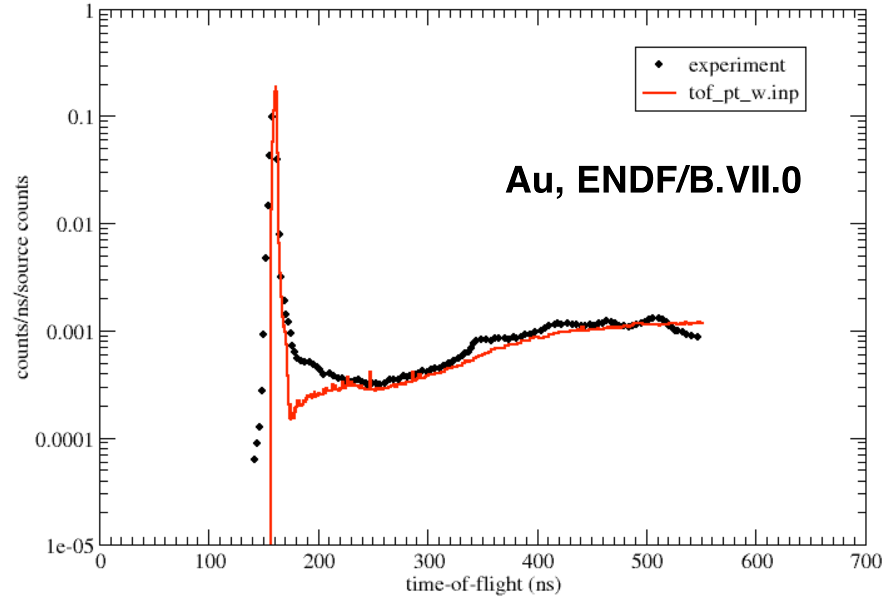
A first look at Si and Cu simulations with ENDF/B.VII.0

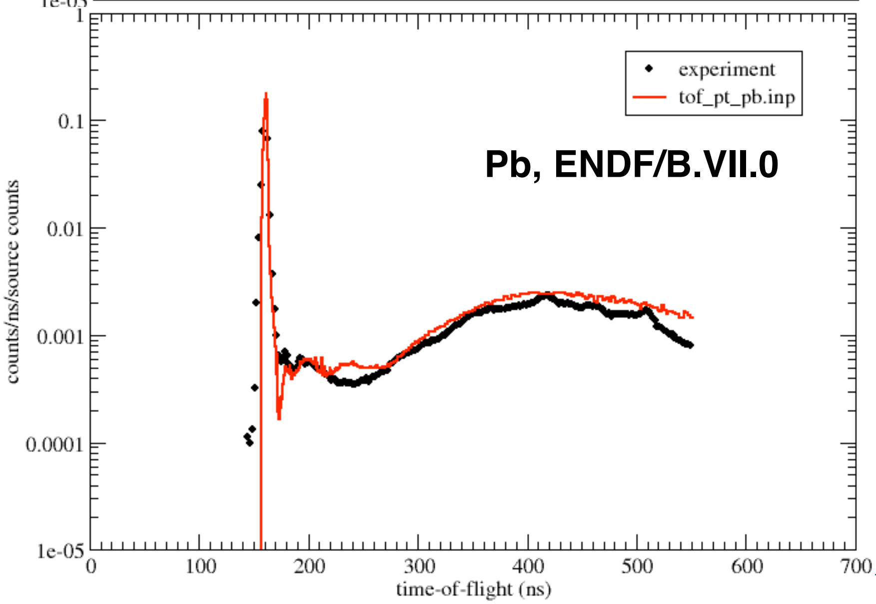




We underestimate the production of 10-12 MeV neutrons for W, Au, and Pb.

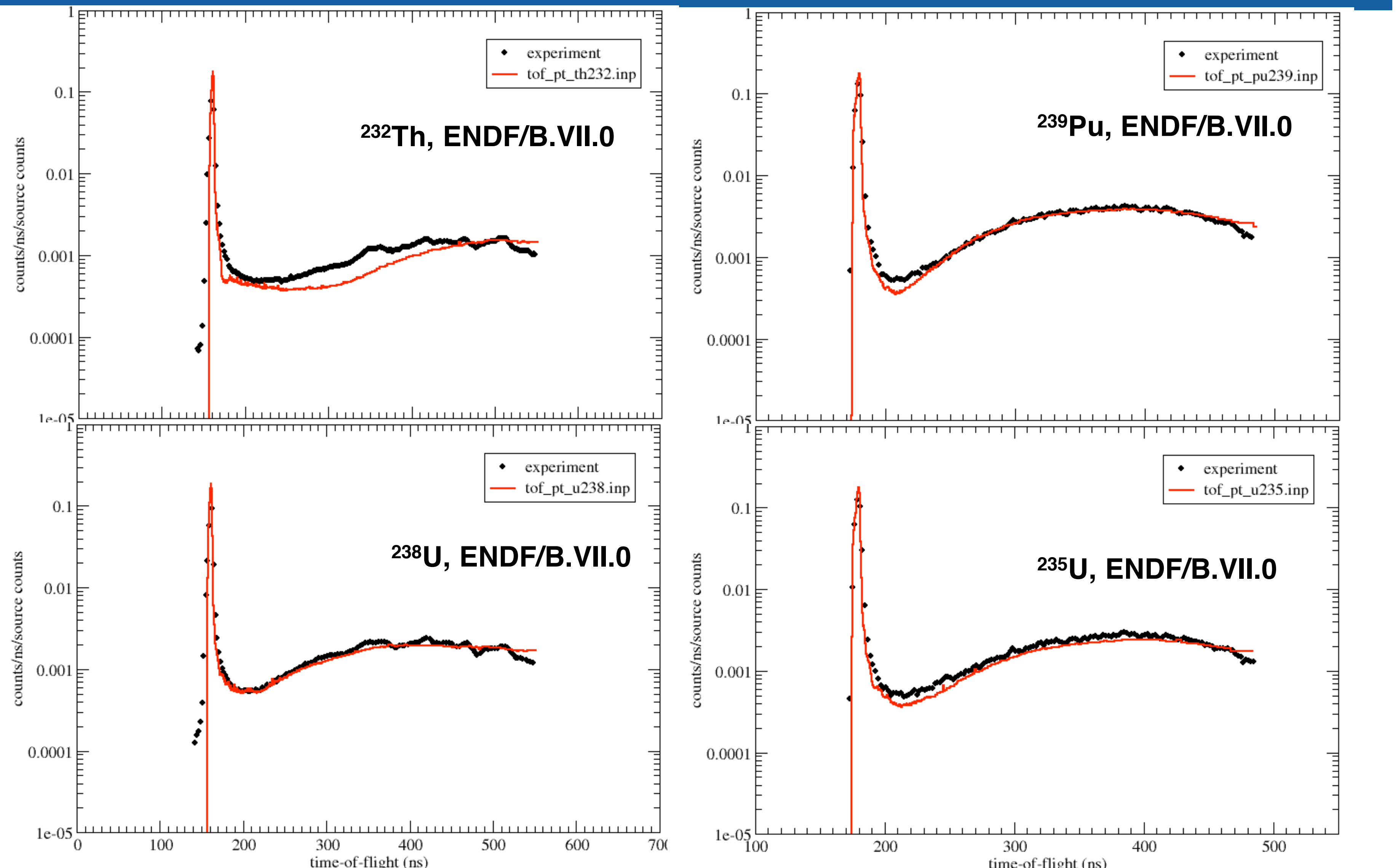




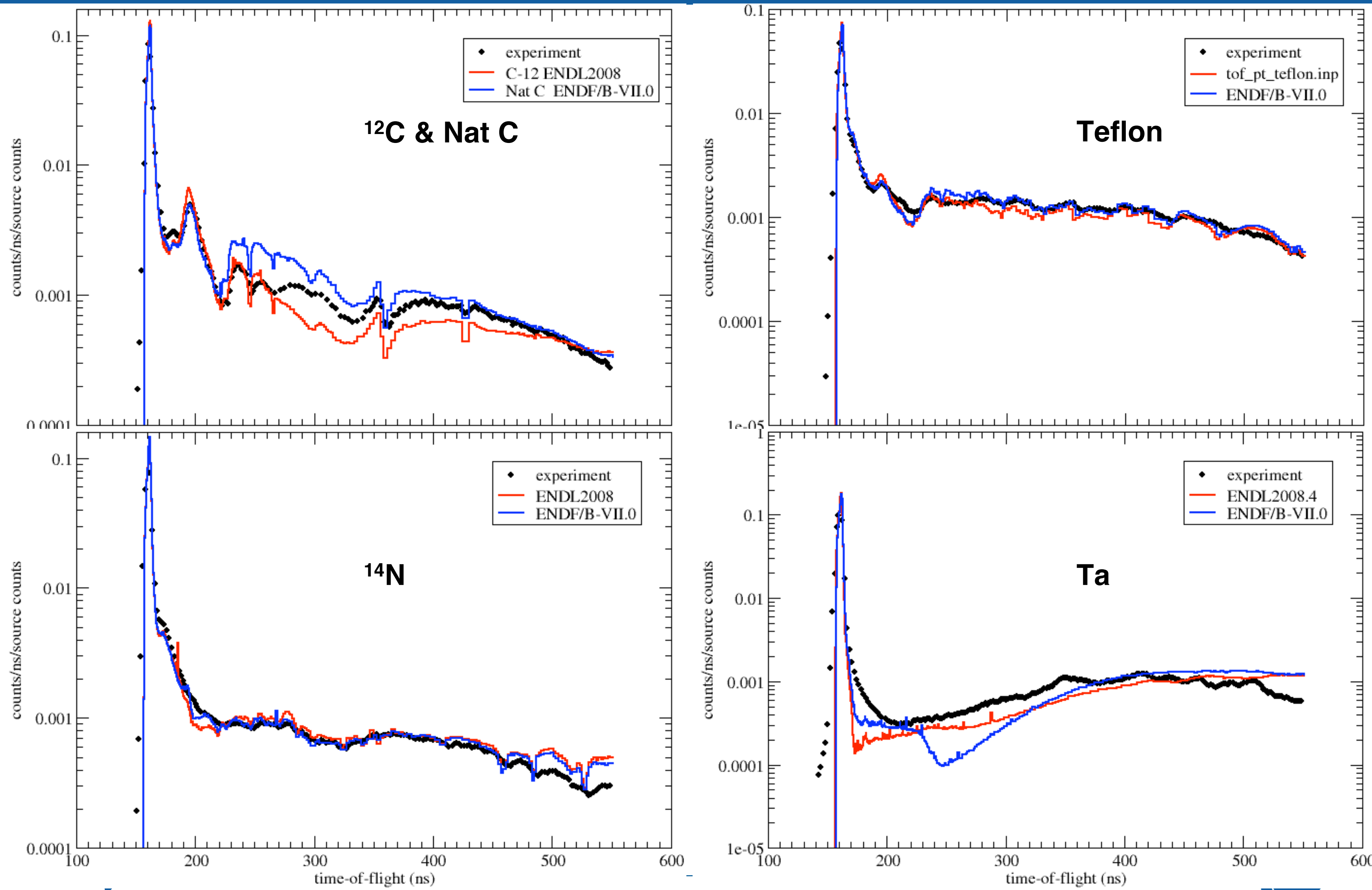


- We are investigating why we underestimate neutron production at energies just below the source energy.

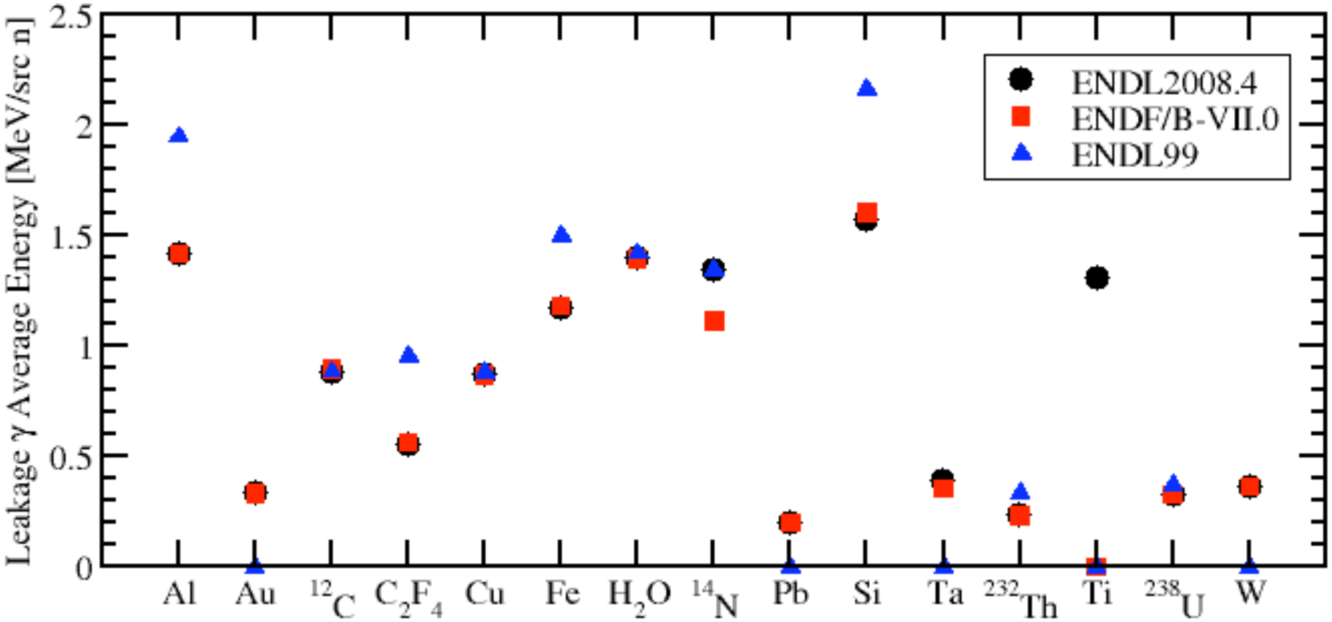
^{232}Th, ^{238}U, and two 1976 experiments for ^{235}U, ^{239}Pu



Differences between ENDL2008 and ENDF/B-VII.0
C, teflon, ^{14}N and Ta



Outgoing gamma spectra as defined by Goldberg et al. (1990)



- Gammas production measured by electron recoil spectra in a NE213 detector
- Mercury cannot transport electrons currently, so compare to Goldberg's 1D simulations
- ENDL2008 performance overall best with exception of ^{19}F & ^{14}N targets
  - ^{19}F targeted for re-evaluation, both ENDL99 & ENDF/B-VII.0 obsolete
  - ^{14}N from ENDF/B-VII.0 acceptable once break-up data translation resolved

Testing has revealed several data problems; these are our recommendations for tackling them

Computational Nuclear Physics

- Reflected critical assemblies:
  - ^{9}Be may need attention
  - Ni, W isotopes need re-evaluation
- Legacy breakup data
  - Short-term: replace LR flagged (n,n') in ^{6}Li, ^{7}Li, ^{14}N, ^{11}B with true double differential data
  - Long term: re-evaluate all four isotopes
  - ^{nat}C: re-evaluate -- this is important material that should have isotopic evaluations and true double differential data
- Diagnose poor performance in pulsed sphere tests:
  - Gamma flux test: ^{19}F, ^{14}N
- Need better $S_{\alpha\beta}$ support in ENDL libraries, LLNL transport codes

We must continue developing new tests;
this is best way to uncover existing problems

New tests to be added this year

- More criticality tests: Red Cullen's fantastic TART test suite
- Fusion Shielding Benchmarks
  - Oktavian spheres
  - FNS
- LANL Traverse measurements