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Neutron capture spectra and other nuclear data plans

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Goal: Improve capture spectra used in transport codes

- **Applications sometimes require accurate simulations of data**
  - Backgrounds
  - Energy conservation
  - Energy and multiplicity distributions per event

- **Very few experiments directly measure QC spectrum**
  - A lot of work to unfold detector response
  - Typically requires isotopically-enriched targets to interpret data
  - I'm still looking for good examples in the literature

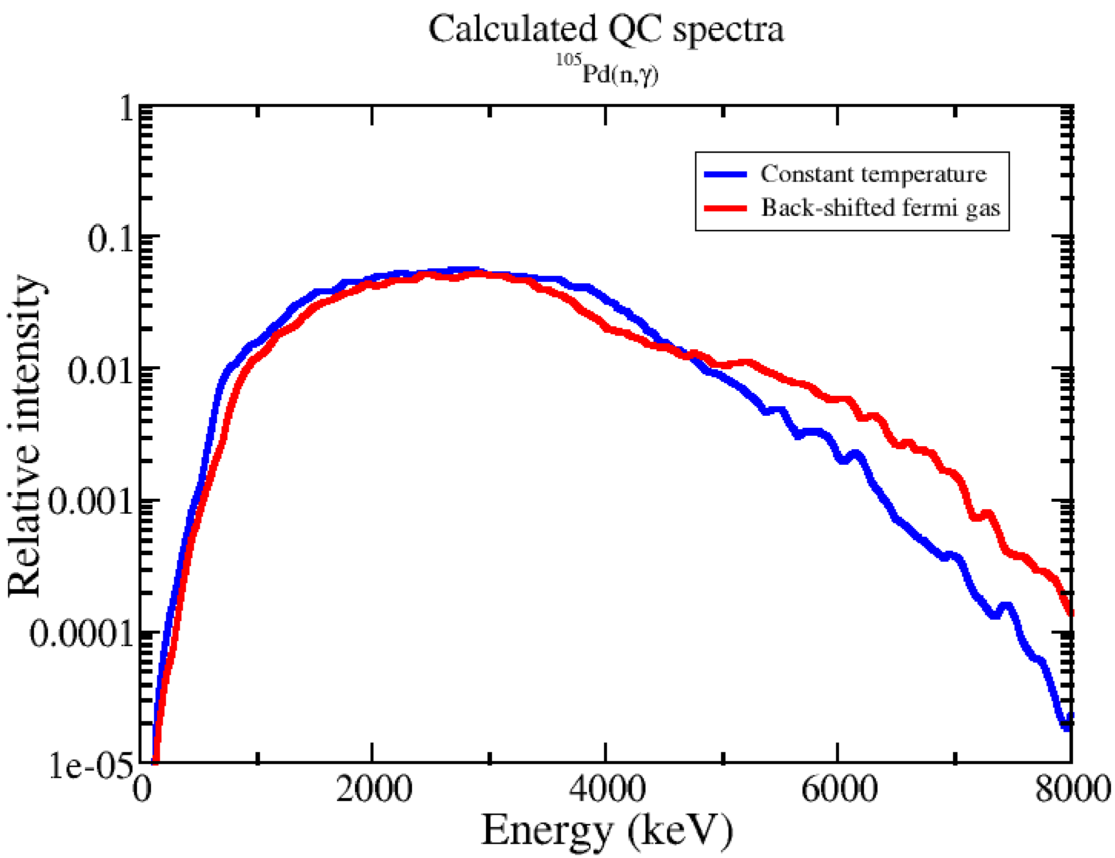
Solution: Model QC spectra

Problem: How do we validate calculations without direct experimental evidence?

The overall plan

- **Develop the γ-ray decay model**
  - γ-ray cascade algorithm from F. Becvar (NIM A417, 434 (1998))
  - Physics input from a variety of sources
- **Validate model against thermal neutron capture gamma-ray data**
  - Gamma-ray lines and relative intensities
    - » Institute of Isotope and Surface Chemistry, Budapest
    - » EGAF: Extensive re-evaluation of all the literature
  - Total partial widths: Γ_γ
- **Demonstrate that new model is predictive**
  - Nuclear spectroscopy: J^π assignments
  - Neutron capture cross sections from γ-ray cross sections
- **Crank out new evaluations for ENDF**
  - Database feeds transport codes such as MCNP

Sensitivity to level density explored



χ^2 **for levels**

- CT: 1.7
- BSFG: 1.7

Γ_γ **Exp. 150(8) meV**

- CT: ≈ 112 meV
- BSFG: ≈ 335 meV

Multiplicity

- CT: 4.3
- BSFG: 4.5

More data may be needed to zero in on QC spectrum

Light isotopes don't have a quasi-continuum

- **Converting EGAF into ENDF for Z ≈< 20**

- **Using current ENDF capture cross sections**
  - Recent data suggests changes for some isotopes
  - Multiplicity per cascade defined as

$$m_i = \frac{\sigma_i^{EGAF}}{\sigma_{(n,\gamma)}^{ENDF}}$$

- **One overall scale factor used to conserve energy**
  - Worst case so far is an ≈ 15% correction

$$Q = A \sum_i m_i E_{\gamma i}$$

Work by Brad Sleaford

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11 isotopes converted and tested to date

Tgt ZA	NK,#	linN.A.	(MugS(eV*Yield)	(Q-S(eV*Yield))	Comments/Status
1001	1	99.98%	2.2263E+06	-0.06%	Ace, Gendf Libraries complete
1002	1	100.00%	6.2502E+06	0.11%	Ace, Gendf Libraries complete
2003	1	0.00%	6.2502E+06	0.11%	
3006	3	0.07589	1.47E+07	-1.030000E-02	Ace, Gendf Libraries complete
3007	3	92.41%	2.0464E+06	-0.66%	Ace, Gendf Libraries complete
4009	12	1	7.02E+06	-3.001541E-02	Ace, Gendf Libraries complete
5010	10	19.82%	6.9402E+06		TBD
5011	9	0.8018	7.20E+06		TBD
6013	13		5.786693E+06	-0.169738	Natural
6012	6	98.89%	5.3922E+06	-9.01%	Ace, Gendf Libraries complete
6013	7	1.11%	6.9920E+06	14.49%	Ace, Gendf Libraries complete
7014	60	99.63%	1.0794E+07	0.34%	Ace, Gendf Libraries complete
8016	4	99.76%	4.2191E+06	-1.84%	Ace, Gendf Libraries complete
8017	20	0.03%	9.0172E+06	-12.06%	Natural
9019	165	100.00%	6.6043E+06	-0.05%	OK
10020	27	90.48%	6.7118E+06	0.73%	TBD
10021	11	0.27%	1.1456E+07	-10.54%	TBD
10022	10	9.25%	5.0577E+06	2.75%	TBD
11023	233	100.00%	6.5101E+06	6.46%	Libraries complete (natural)
12024	35	78.99%	7.3899E+06	-0.81%	In Process
12025	206	10.00%	1.0927E+07	1.49%	In Process
12026	41	11.01%	6.5472E+06	-1.61%	In Process
13027	230		7.55E+06	2.25%	Ace Gendf Libraries complete
14028	46	92.23%	1.7363E+07	-8.98%	Ace, Gendf Libraries complete
14029	98	4.68%	1.1288E+08		TBD
14030	38	3.09%	7.4716E+06		TBD
15031	158	100.00%	7.3497E+06		TBD
16032	101	95.02%	8.4862E+06		TBD
16033	249	0.75%	1.0342E+07		TBD

Example: ^{27}Al(n,γ) EGAF spectrum in ENDF format

```
ENDF/B- VI Ev aluat i on,  Augus t  2004 ,  R.  F. Fi  r esto  ne (L  BNL)          12 00 14 51   13
            D.  Mcnabb,   B. W .  Sl eafor  d  (LL NL)                            120 0  1451   14
                                                                                  12 00 14 51   15
  The p  r ompt  gamma -ray   spec  t rum f  or th  ermal  ra diati  ve ca  pture   1   200  1451   16
(MF  12,   MT 1 02) h  as be  en up  dated   with   new e  xperi  menta  l  dat  a.[ Fi ]  12 00 14 51   17
                                                                                  12 00 14 51   18

REFERENCE                                                                        12  00 14 51   21
                                                                                  12 00 14 51   22
 [ Fi ]  D    ata   deriv  ed fr  om th  e  Eval uated   Gamma -ray   Acti  vatio  n  Fil  e 1200  1451   23
   (EGAF) as    desc  r ibed   in "  Databa  s e of   Prom pt Ga  mma R ays f  r om S l ow 12 00 14 51   24
   Neut  r on C  aptur  e  for   Elem ental   Analy  s is",   R.B.   Fire  s tone  ,       1200 1451   25
   H.D.  Choi, R  . M. L  i ndst  r om,  G.L.   Molnar  ,  S.F .  Mughabg  hab ,         1200 1451   26
   R.  Pa viott  i -Cor  cuera  ,  Zs.  Revay,   V.  Zerkin,   and  C.M.  Zhou ,         1200 1  451   27
   IAEA  TECDOC, i  n  pre  s s.                                                 12   00 14 51   28
                                                                                  12 00 14 51   29

 1 . 3027 00+4  2.674  975+1            1          0          291         013  25121 02275 19
 0 . 0000 00+0  0. 00000 0+0            0          0            1       171325 121022 7520
          17           2                                                  13 25121 02275 21
 1 . 0000 00-5  2.230  130+0  1.00  0000+4  2.23  0130+ 0  1.0  00000 +5 2.  23000 0+013 25121 02275 22
 5 . 0000 00+5  2.450  000+0  1.00  0000+6  2.45  0000+ 0  2.0  00000 +6 2.  47000 0+013 25121 02275 23
 3 . 0000 00+6  2.500  000+0  4.00  0000+6  2.55  0000+ 0  6.0  00000 +6 2.  61000 0+013 25121 02275 24
 8 . 0000 00+6  2.840  000+0  1.00  0000+7  2.95  0000+ 0  1.2  00000 +7 2.  98000 0+013 25121 02275 25
 1 . 4000 00+7  3.050  000+0  1.70  0000+7  3.36  0000+ 0  2.0  00000 +7 3.  91000 0+013 25121 02275 26
 2 . 0000 01+7  0.000  000+0  1.50  0000+8  0.00  0000+ 0                            13 25121 02275 27
 7 . 7240 26+6  0.000  000+0            0          2            1         613  25121 02275 28
            6          2                                                  13 25121 02275 29
 1 . 0000 00-5  2.874  819-1  1.00  0000+4  2.87  4819- 1  1.0  00000 +5 0.  00000 0+013 25121 02275 30
 2 . 0000 00+7  0.000  000+0  2.00  0001+7  0.00  0000+ 0  1.5  00000 +8 0.  00000 0+013 25121 02275 31
```

V&V: ^{27}Al irradiated with thermalized Cf neutrons

Outlook is good for delivering new thermal neutron capture spectra one year from now

- Validating our model against data
  - Experimental QC spectra would be useful
  - Γ_γ widths may be enough to select "best" model
- Model is predictive
- Systematic uncertainties in the computed QC spectrum due to
  - Level density
  - Strength functions
- Need to add more test cases before confident in prescription

Future plans for improving photon production

- Non-thermal neutron capture spectra
- Inelastic scattering photon production
- Decay spectra
- Joint LBNL/LLNL website targeted to homeland security personnel interested in these issues

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Goal: Improve transport simulation capability for new radiochemical diagnostics (actinides)

- **Add physics of low-energy neutron scattering to nuclear data code libraries to improve fidelity of (n,γ) simulations**
  - **MCAPM**
  - **NDF**

- **Collaborate with LANL on best estimates of actinide production/depletion cross sections *with uncertainties***
  - **Good fission cross sections are key for fast neutrons**
  - **Good capture cross sections are key for slow neutrons**

We bring an experimental focus to this collaboration

Fission and capture cross sections are hard to predict theoretically

$$\sigma_r = \sigma_{(n,f)} + \sigma_{(n,n')} + \sigma_{(n,2n)} \left(+\sigma_{(n,\gamma)}\right)$$
$$= \pi (R + \mathrm{D})^2 \left(1 - e^{-\alpha}\right)$$

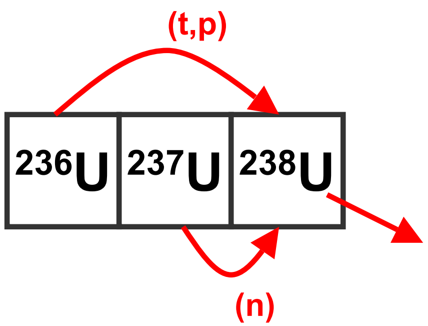
- **6-parameter fit with dependence on E_n, N, Z good to ≈1%**
  - **2 parameters for R**
  - **4 parameters for α**

- **σ_r for nuclei with no data to 3-4% for fast neutrons**
  - **McNabb et al., submitted to NSE & ND conference**
  - **Follow up work in progress**

Fission cross sections are the missing link
Need good model of functional shapes of (n,n’) and (n,2n)

Two-prong effort on fission data

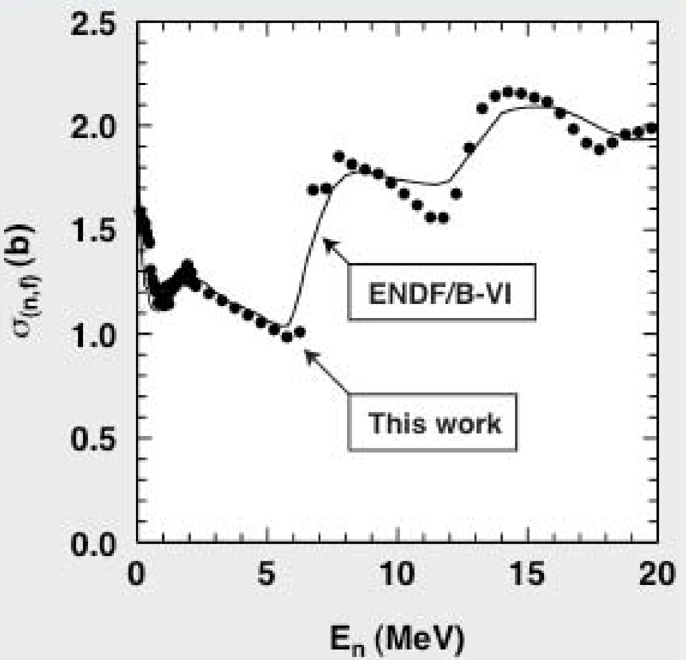
- **Analyze old transfer data for E < 2.2 MeV**
  - Extend to 14 MeV w/ theory
- **Obtain new data with improved technology**
  - Extend experiments to higher energies
  - Improve understanding of errors



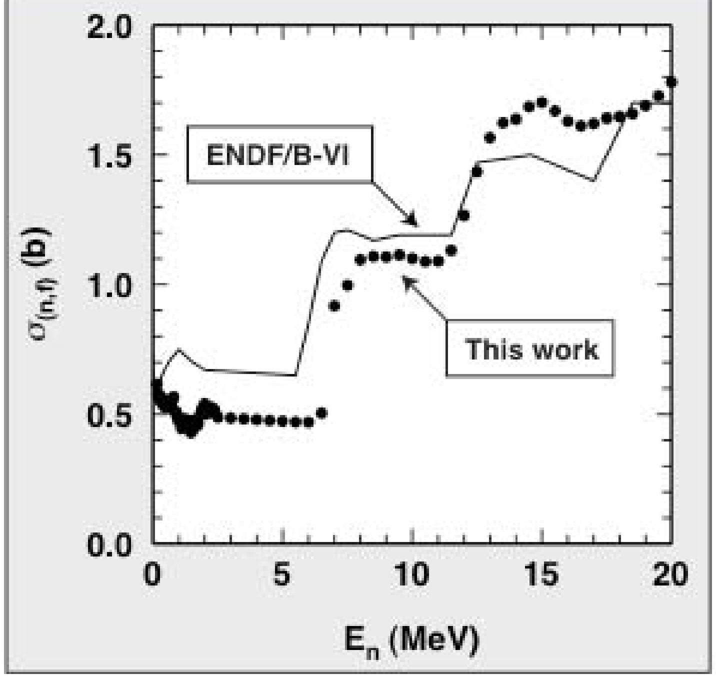
Both efforts use data from "surrogate" reactions

Preliminary extension of (n,f) to E_n = 20 MeV

Validation: ^{235}U(n,f) cross section



Prediction: ^{237}U(n,f) cross section

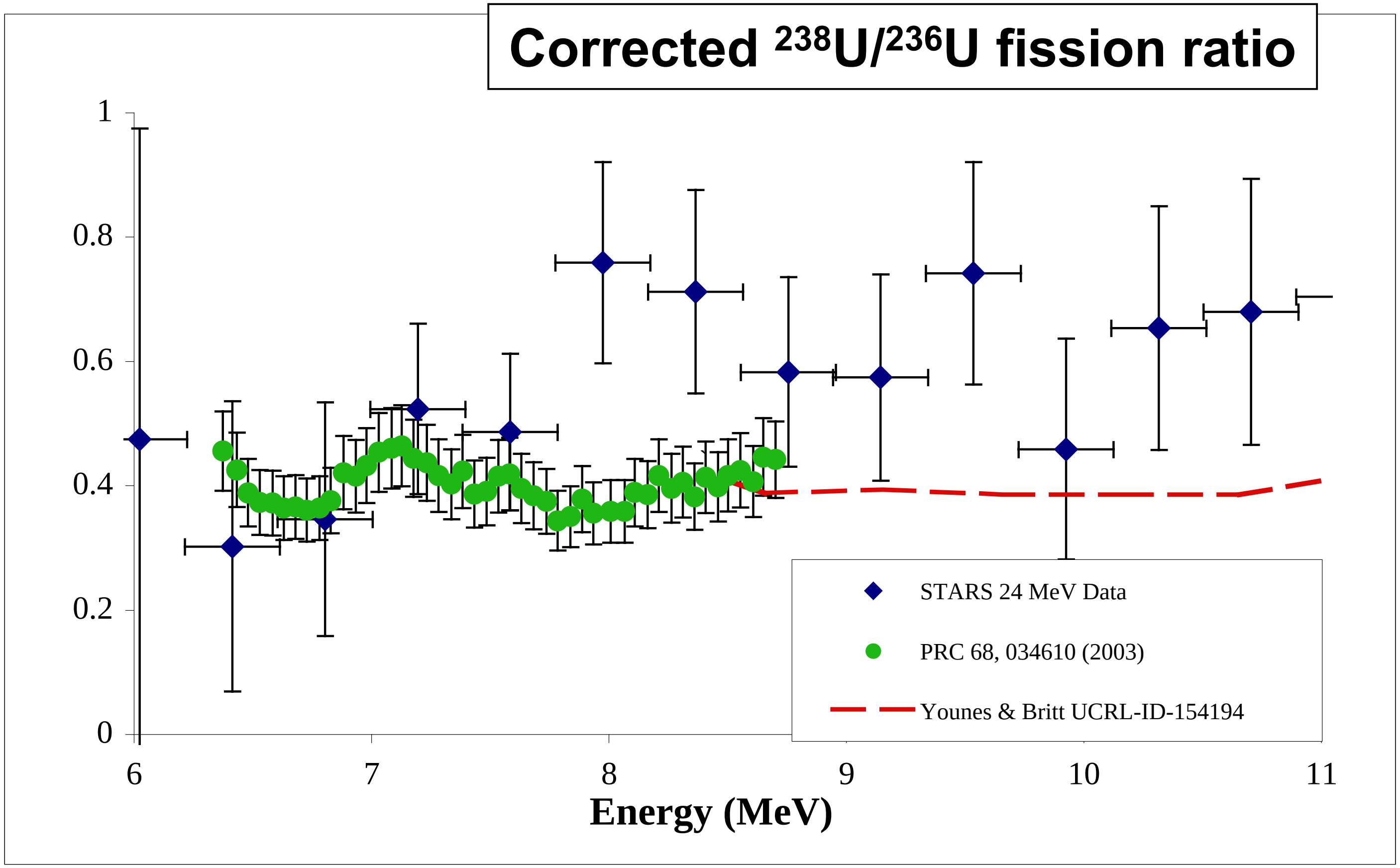


- Surrogate-data estimate of ^{235,237}U(n,f) currently limited to E_n < 2.2 MeV
  - – use linear extrapolation for 1st-chance fission
  - – use measured $^{A-1}$U(n,f) for 2nd+3rd-chance fission
- W. Younes et al., UCRL-ID-154194 (2003)

Looks promising, but need improved fission model
⇒ predictions up to 20 MeV entirely from surrogate data

Validation of the surrogate technique for Actinides: $^{236,238}U(d,d')$ with STARS - May 2004

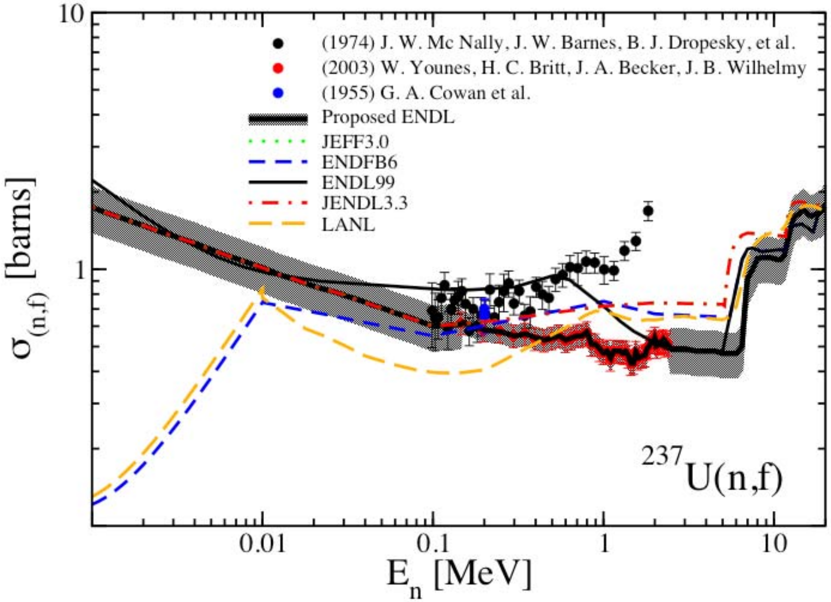
Work by L. Bernstein, J. Church, L. Ahle, J. Punyon

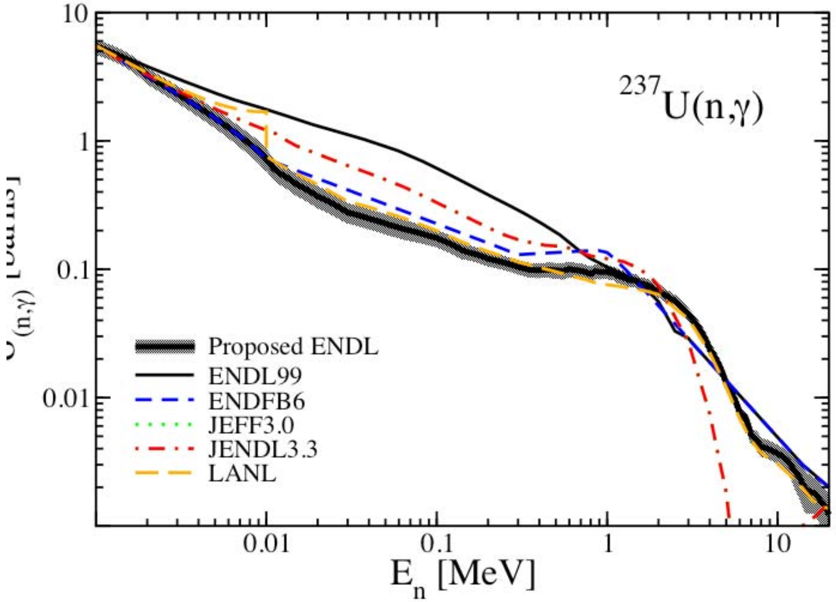


PRELIMINARY ratios in agreement with W. Younes et. al.
^{238}U analysis (non-ratio) still in progress

Work by David Brown, UCRL-TR-202393

Generating the starting point for a global fit





First-pass results for $^{232\text{-}241}$U cross sections delivered:

- **Adopted model calculations from Japan, Europe, US**
- **Modified results in key areas based on data, sum rules**
- **Estimated model uncertainties in a crude fashion**

"I'm pleased to see that uncertainties are being added to the data."
-- C. McMillan. B-Div Leader

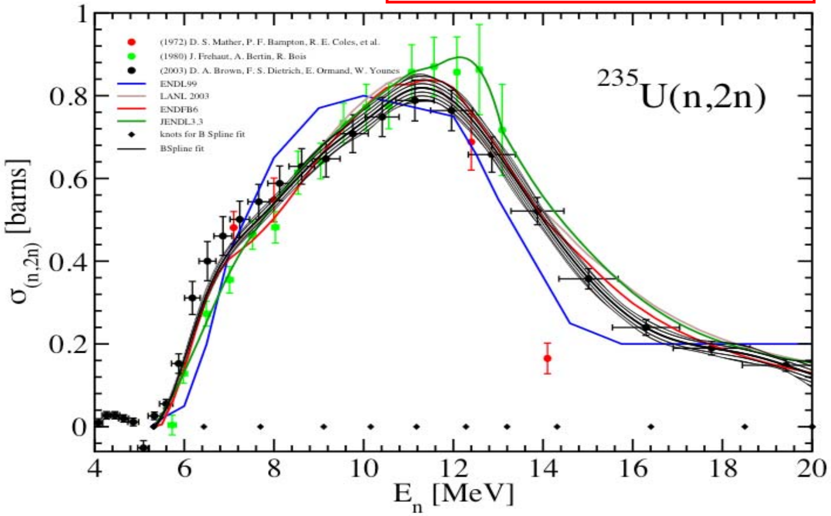
Physics & Advanced Technologies

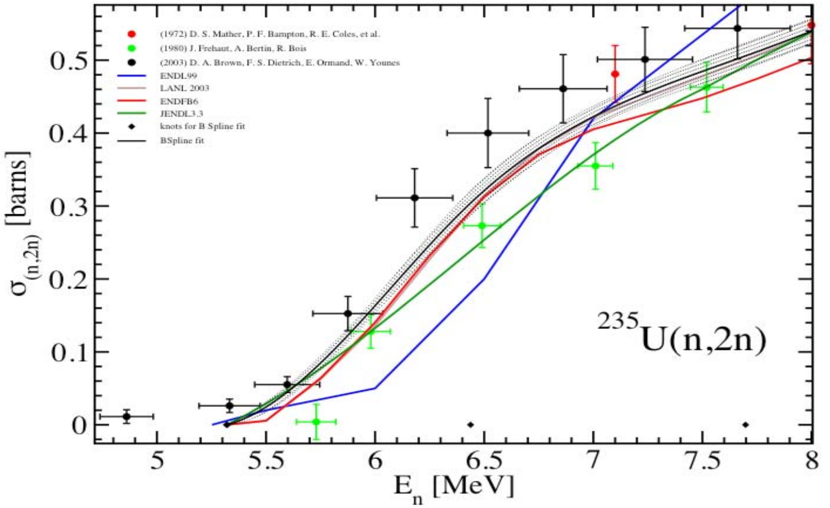
Constrained fits to evaluated data, uncertainties

Work by David Brown

- **Production and depletion of actinide isotopes**
  - **Forensic signatures**
  - **Uncertainties required**

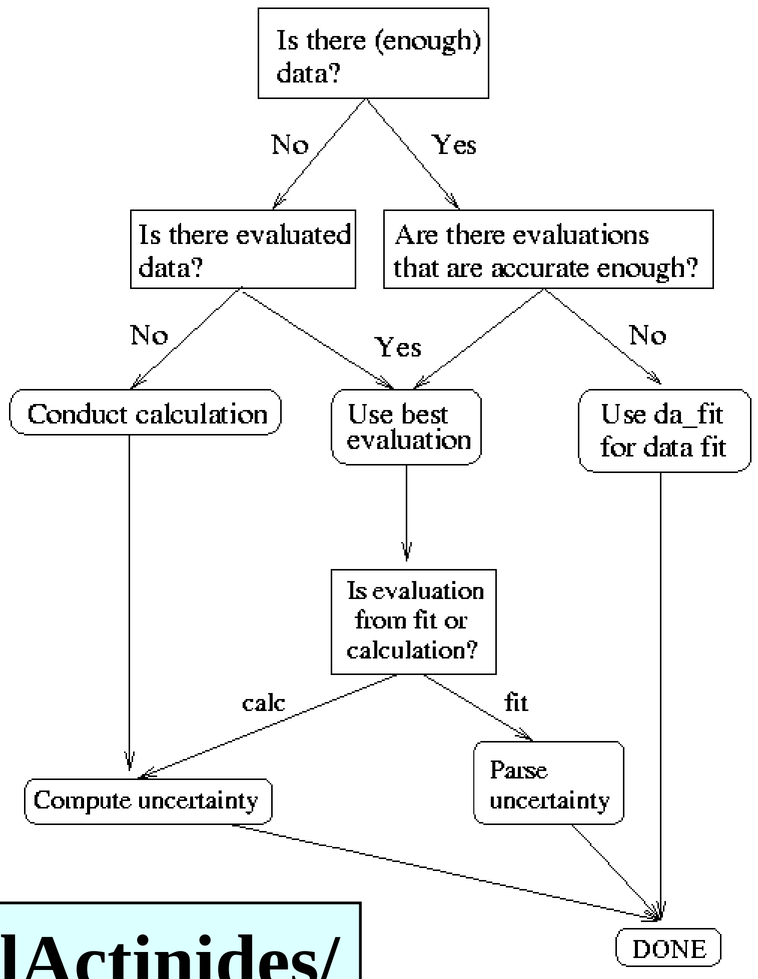
- **Simultaneous fit to actinide cross section data**
  - **Data-driven**
    - » **Covariances included**
  - **Theoretical assumptions**
    - » **Explicit constraints**
  - **Uncertainties intrinsic**





Automating as much as we can to generate first-pass estimate for all nuclei

- *x4i* to parse exp. data
- *fete* to parse ENDF/B data
  - prelim. ENDF/B-6, JEFF3.0, JENDL3.3
- Constrained, generalized least-square spline fitter



http://nuclear.llnl.gov/CNP/allActinides/

New issues & future directions

- We're close to having a first-pass cross section set
  - Now our goal is to "do it right" (global fit)
- We are excited about surrogate fission effort
  - Will require a sustained multi-year effort
- Working toward more involved in DANCE (n,γ) measurements

NADS 1.4 & 1.5 (Changes from last year)

- Rewrote 2-D plotting
  - Publication quality graphics
  - More control over look and feel (similar to xmgrace)
  - Faster plotting with large data sets
  - Plots uncertainties
  - Preferences can be saved
- Added EXFOR cross section data
- Improved computational features
  - Merge EXFOR data sets
  - Save/load computation sessions
  - Commands history
  - Some 2-D data (vector) math added
- New table features
  - Tab-delimited text file may be read in
  - Tables can be edited and saved or replotted
- Modified server start-up procedure
  - Starts up in 30 seconds, loads data into memory as requested
  - Will help us deal with lost port problem / crashes