LANL-EDA R-matrix cross section evaluations

Charged-particle reactions

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CSEWG-US National Nuclear Data Week
Brookhaven National Laboratory
2019 November 4-8

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

LA-UR-19-31035

Outline

- **LANL cross section evaluation codes**
  - EDA5: Simultaneous fit of all reaction/scattering data in R-matrix approach
  - SPECT: Spectra calculated in resonance model with auxiliary code/input from EDA5
- **CSEWG evaluation criteria**
  - LANL light-element data pipeline
  - Evaluation revision criteria
  - Recommendations for ADVANCE CI/CD [git repos]
- **New ENDF-6 formatted evaluations**
  - `p-002_He_004.endf`
  - `d-002_He_004.endf`
  - `a-002_He_004.endf`
- **Ongoing work**

LANL-EDA code

- **R-matrix formalism [Wigner(1947)]**
  - Unified description of many reactions
  - Ensures unitarity & probability conservation
- **Capabilities**
  - Any projectile: n, p, D, T, ^{3}He, α, …
  - Any target: H, He, Li, Be, B, C, N, O, F, …
  - All data fit ***together, at the same time***
    - Elastic, inelastic, rearrangement, breakup, capture
  - All observables
    - Cross sections: elastic, reaction, total
    - Angular distributions/excitation functions
    - Polarization observables
    - Spectra 2➔3, 2➔4
    - Capture/electromagnetic
- **High-fidelity fit:**
  - Typical chi-squared: χ^2/dof ~ 1.2 – 1.5
  - And, yes, we generate COVARIANCES!

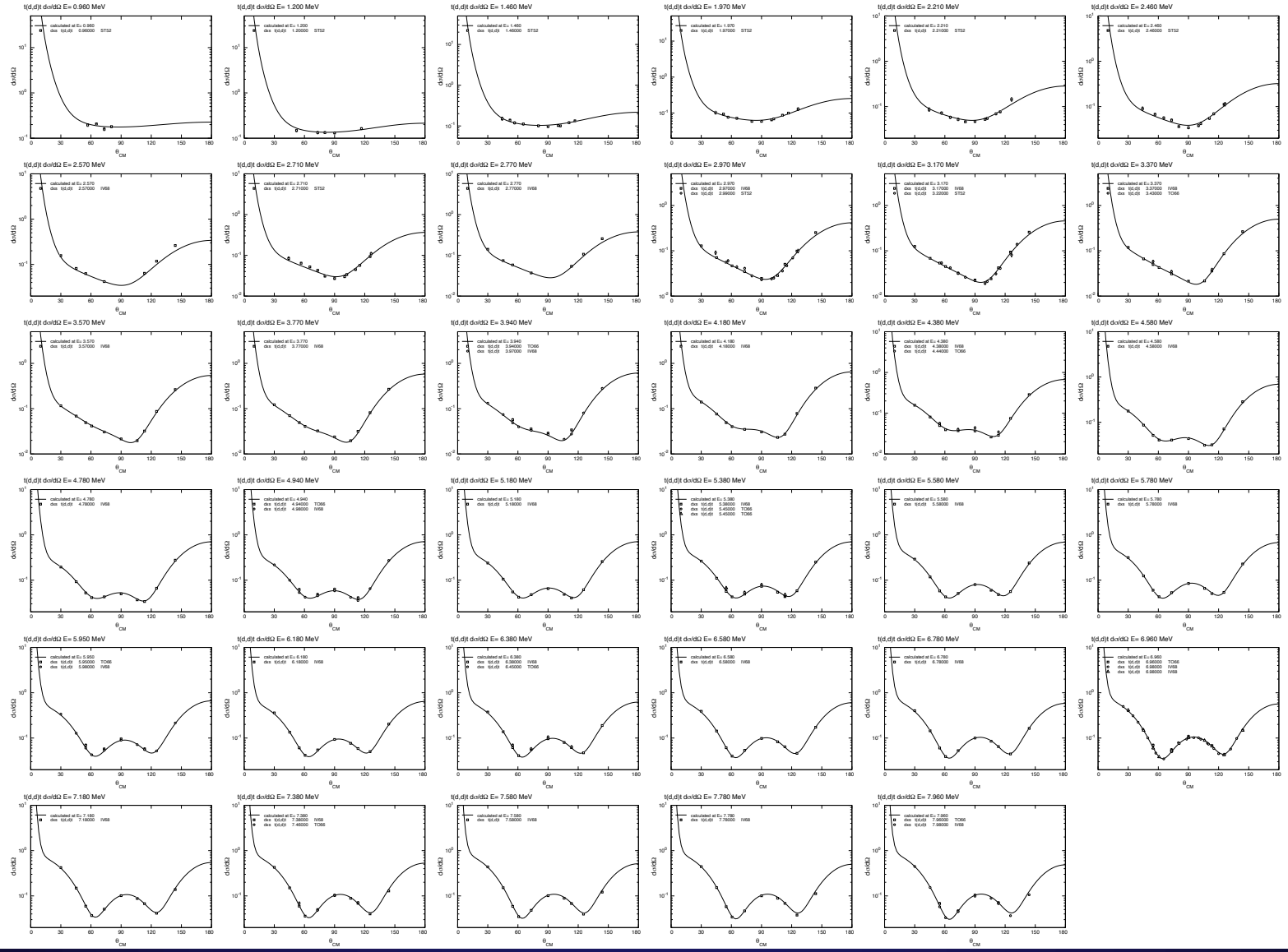
Channel	a_c (fm)	l_{max}
t+^{4}He	4.02	5
n+^{6}Li	5.0	3
n+^{6}Li*	5.5	1
d+^{5}He	6.0	0

Reaction	Energy Range (MeV)	# Pts.	Observables
^{4}He(t,t)^{4}He	E_t=0 - 14	1661	σ(θ), $A_y(t)$
^{4}He(t,n)^{6}Li	E_t = 8.75 - 14.4	37	σ_{int}, σ(θ)
^{4}He(t,n)^{6}Li*	E_t =12.9	4	σ(θ)
^{6}Li(n,t)^{4}He	E_n = 0 - 4	1406	σ_{int}, σ(θ)
^{6}Li(n,n)^{6}Li	E_n = 0 - 4	800	σ_T, σ_{int}, σ(θ), $P_y(n)$
^{6}Li(n,n')^{6}Li*	E_n = 3.35 - 4	8	σ_{int}
^{6}Li(n,d)^{5}He	E_n = 3.35 - 4	2	σ_{int}
Total		3918	13

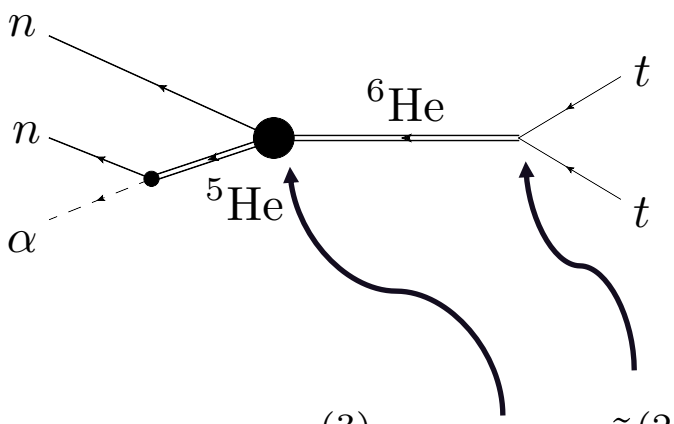
- **Unified, simultaneous fit**
  - describe all data together
  - fit quantum mechanical amplitudes, not cross sections
- **Built-in Quality Assurance**
  - Normalization constrained
    - Weed-out underestimated exp'l uncertainties
- ***Superior to single-channel or polynomial fitting***

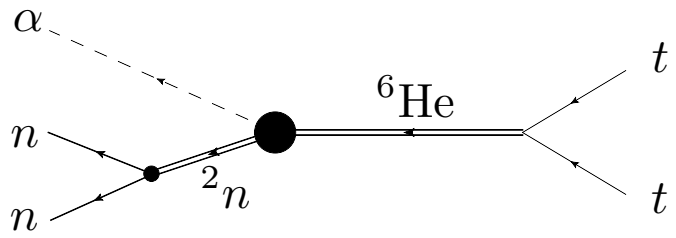
^{7}Li compound system evaluation

Angular distributions ^{4}He(t,el)

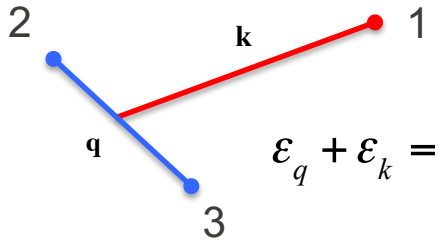


Spectra (SPECT code) resonance model





$$T^{(3)}_{\mathbf{qkk_0}} = c_\lambda(\mathbf{q})\tilde{T}^{(2)}_{\lambda\mathbf{kk_0}}$$



$\varepsilon_q + \varepsilon_k = \varepsilon =$ total c.m. energy

$$c_\lambda(\mathbf{q}) = \sqrt{\frac{\hbar^2\Gamma_\lambda(\varepsilon_q)}{2\pi\mu_{23}q}}\left[\varepsilon_\lambda + \Delta_\lambda(\varepsilon_q) - (\varepsilon_q) - \tfrac{i}{2}\Gamma_\lambda(\varepsilon_q)\right]^{-1} \mathrm{e}^{-i\phi_{\tilde{l}}}\, Y^0_{\tilde{l}}(\hat{\mathbf{q}}),$$

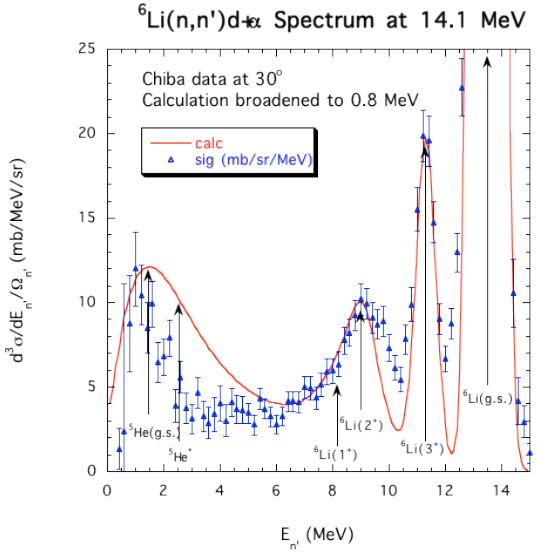
$$\tilde{T}^{(2)}_{\lambda\mathbf{kk}_0} = \sum_{Js'l'sl} Y_{\lambda Js'l'}(\hat{\mathbf{k}}) O^{-1}_{l'}(k) R^{\bar{L}}_{\lambda s'l'sl}(\varepsilon) O^{-1}_{l}(k_0) Y^*_{Jsl}(\hat{\mathbf{k}}_0)$$

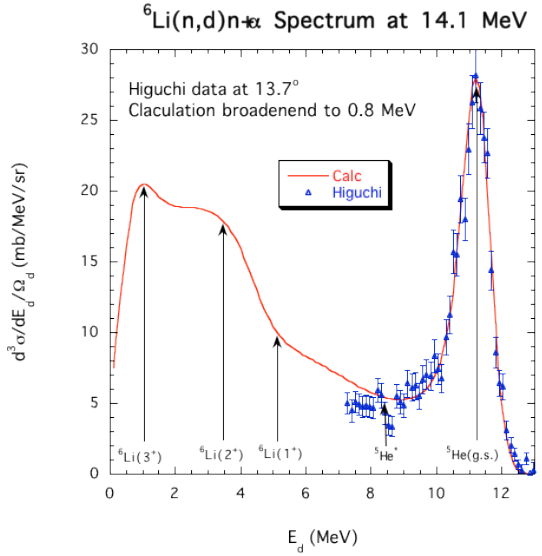
$$\frac{d^3\sigma}{d\mathbf{k}} \propto \int d\mathbf{q} \left|T^{(3)}_{\mathbf{qkk}_0}\right|^2 \delta(\varepsilon_q + \varepsilon_k - \varepsilon)$$

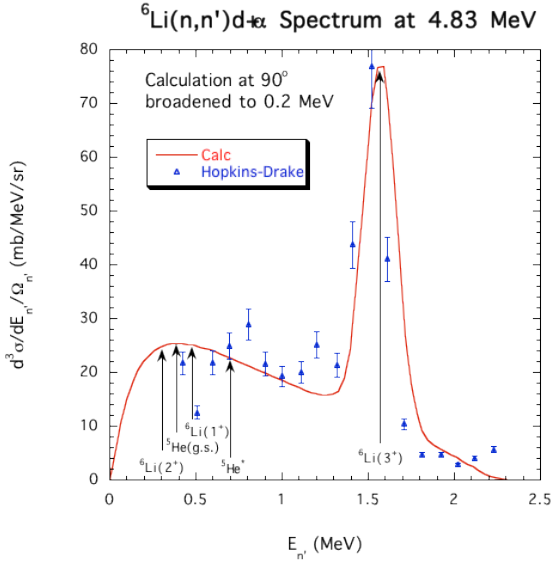
$$\bar{L}_{l'}(\varepsilon) = \frac{\gamma_\lambda^2}{\pi}\int_0^\varepsilon d\varepsilon_q L_{l'}(\varepsilon - \varepsilon_q) \frac{P_{\tilde{l}}(\varepsilon_q)}{\left|\varepsilon_\lambda - \varepsilon_q - \gamma_\lambda^2(L_{\tilde{l}}(\varepsilon_q) - \varepsilon)\right|^2}$$

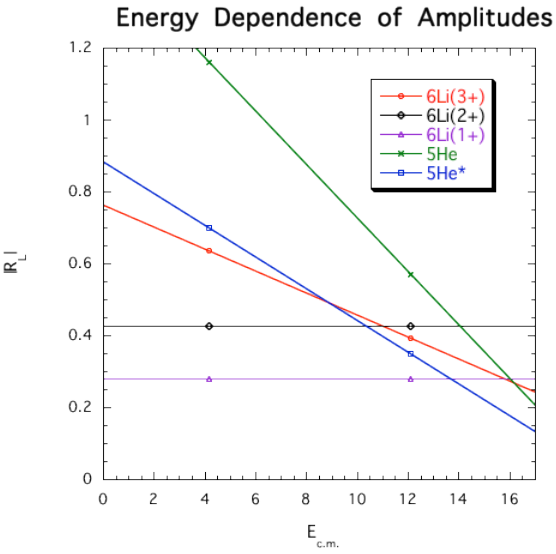
^{6}Li(n,n') fit spectra

- **Neutron-inelastic & deuteron spectra**
- **Subset of available data:**
  - Chiba (1982) @ 14.1 MeV
  - Higuchi (1982) @ 14.1 MeV
  - Hopkins (1968) @ 4.83 MeV
- **Assume linear energy dependence R_L**
  - *Ad hoc;* full energy dependence calculable
- **Resonance structure**
  - recoiling compound system (^{6}Li, ^{5}He)
  - distinct from phase space
    - Featureless, 'bubble' structure



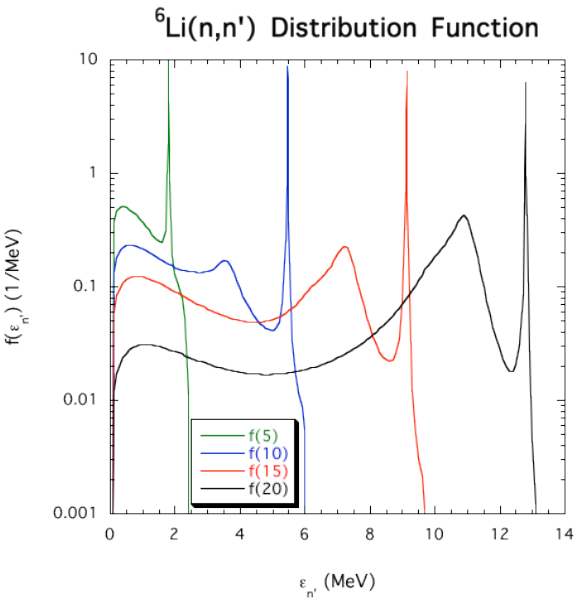


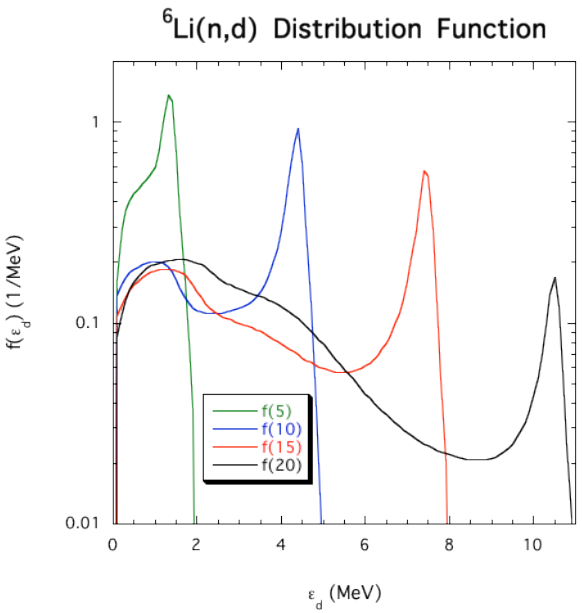


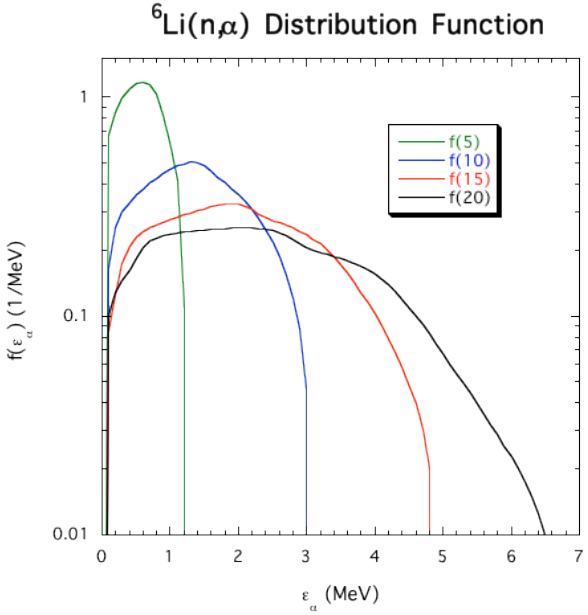


n+^{6}Li CP secondary distributions

Energy dependence







LANL evaluation data pipeline

- **Cross section evaluation**
  - Include all available data [publications, EXFOR/CSISRS, direct comm's, etc.]
    - Check publications for obvious errors/mistakes [lab/cm, norm, units, ...]
    - Extract systematic/statistical errors from publication
    - Individual data points with X^2/DOF > 10. excluded
  - Initialize fit parameters
    - Varied parameters: level energies, reduced widths
    - Theoretical regulators (not *generally* varied): boundary conditions, channel radii
    - From previous evaluations or educated guess
  - Optimize chi-squared (X^2) function
    - Solution determined at local X^2/DOF minimum
    - Determines covariance matrices for all observables via analytic derivatives
- **Processing**
  1. EDA5 → ENDF-6 via EDA-auxillary code
  2. ENDF-6 checking via NNDC (Dunford) ENDF-6 Utility codes
  3. ENDF-6 → NDI (LANL in-house multigroup)
  4. ENDF-6 → ACE (continuous energy/MC) format via NJOY2016

Evaluation revision criteria

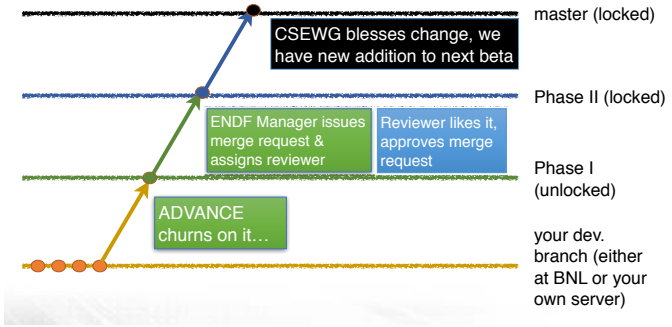
- **Improvement to existing LANL evaluations welcome**
  - Primary concern: eliminate evaluation 'gaps'
    - gaps in recommended energy range $0 < E < 20$ MeV (higher for some)
    - gaps in reactions available (spectra, capture, etc.)
- **Review criteria for evaluation revisions**
  - For reactions without existing evaluation
    - describes the available data well χ^2/dof ~ 1—2
    - covers recommended energy range
    - ENDF-6 compliant
  - For reactions with existing evaluation
    - "complete" (as above)
    - accepted for extension of energy range (appended to existing evaluation)
    - ***substantial*** improvement over existing evaluation requires
      - improved fidelity of data fit
      - improved method/approach of proposed eval.
        - » better theory; simultaneous description of more data; etc.

NB: simpler approaches (such as single-channel curve fitting) offering substantially improved description of data can be accepted

Recommendations for ADVANCE CI/CD (git repository)

(Personal opinion, not nec. those of LANL)

- **Evaluation chair's current (if informal) policy**
  - "the lab that had made the current ENDF file has the responsibility to assess its accuracy/deficiency - as informed by their own knowledge and by knowledge and input from the other lab suggesting alternatives/updates" *–M. Chadwick 2018 Oct*
- **Recommendation #1**
  - Proposed modifications (replacement, extension, correction, ...) must be reviewed by existing evaluation's evaluators, if at all possible
- **Timeline**
  - To give reviewers sufficient time to review proposed modifications and avoid last-minute efforts to replace existing evaluations
- **Recommendation #2**
  - well in advance (3-4 months) of CSEWG
    - Deadline for Phase I submissions (locked after)
  - Previous file evaluator (Reco #1) must approve
    - Final approval by exec-committee requiring 2/3
      - (or something like that)



LANL Light Element Evaluations

	H1	H2	H3	He3	He4	Li6	Li7
n	VIII.0	VII.1	VII.1	VII.1	VII.1	VIII.0	VII.1
p	VII.1	VII.1	VII.1	VII.1	**2020***	VII.1	2001**
d		VII.1	VII.1, 2018	VII.1	**2020**	VII.1	2003**
t			VII.1	VII.1	2011*	VII.1	--*
^{3}He				2001	2011*	VII.1	--
α					**2020***	--	--

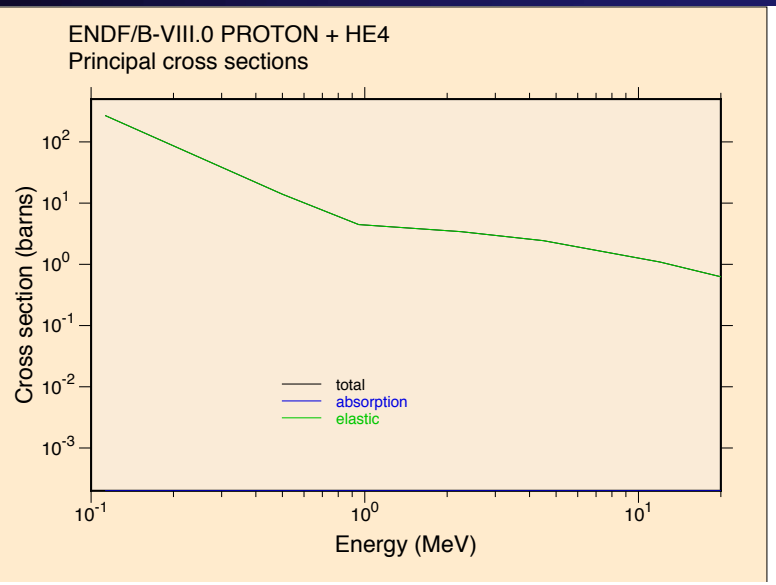
- **Roman numerals refer to ENDF versions**
- **2011: not in ENDF/B-VIII.0**
- **2020: recent submissions "ENDF/B-VIII.b1"**

* Nuclei for which LLNL evaluations have been put into ENDF/B-VIII.0

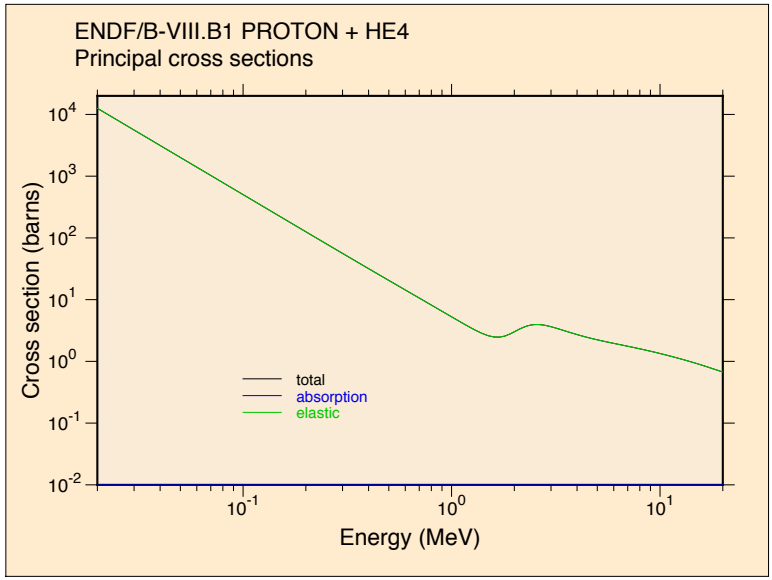
**Nuclei for which LLNL evaluations replaced existing LANL evaluations in VIII.0

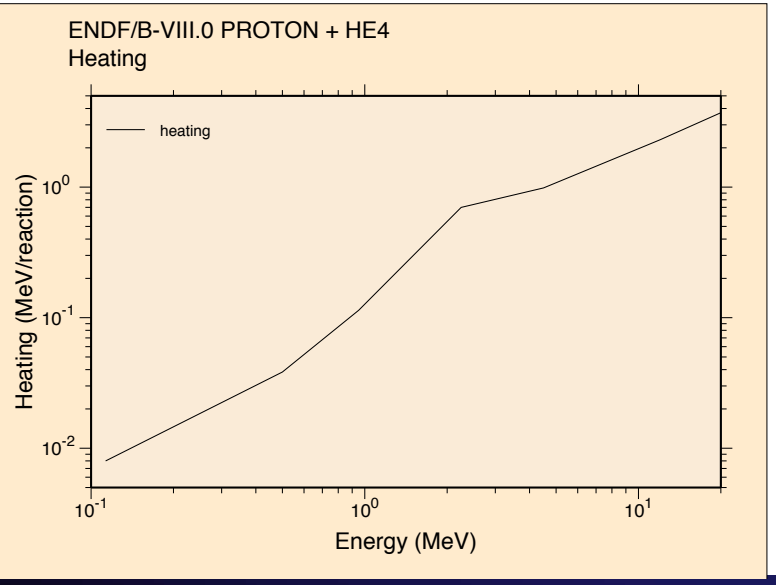
New ENDF-6 evaluations

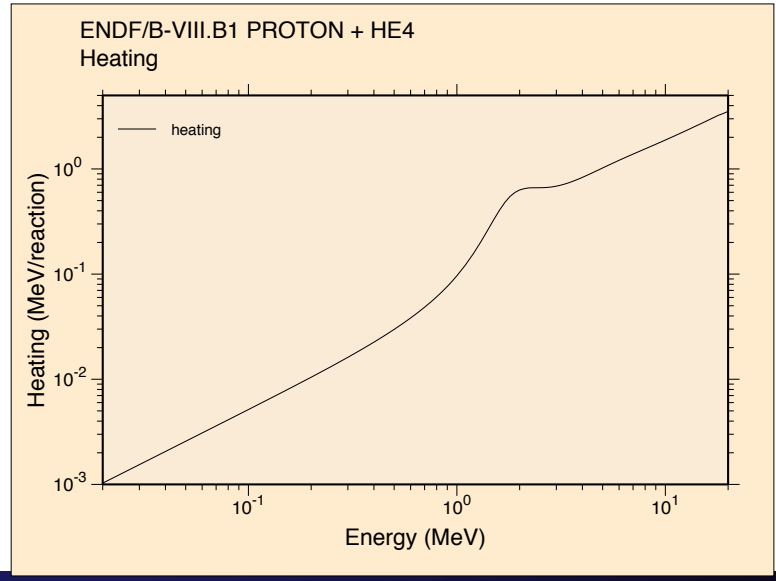
1) *p*+α: ENDF/B-VIII.0 (left) vs. ENDF/B-VIII.b1



Diff x-axes







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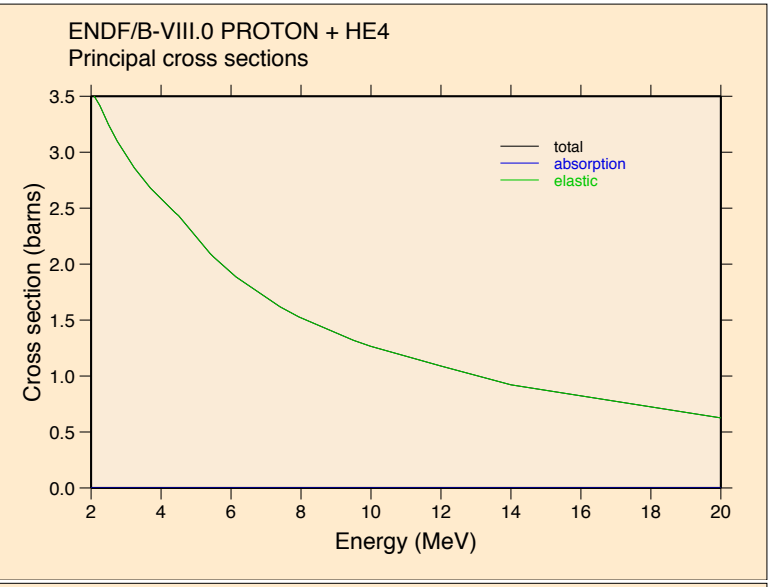

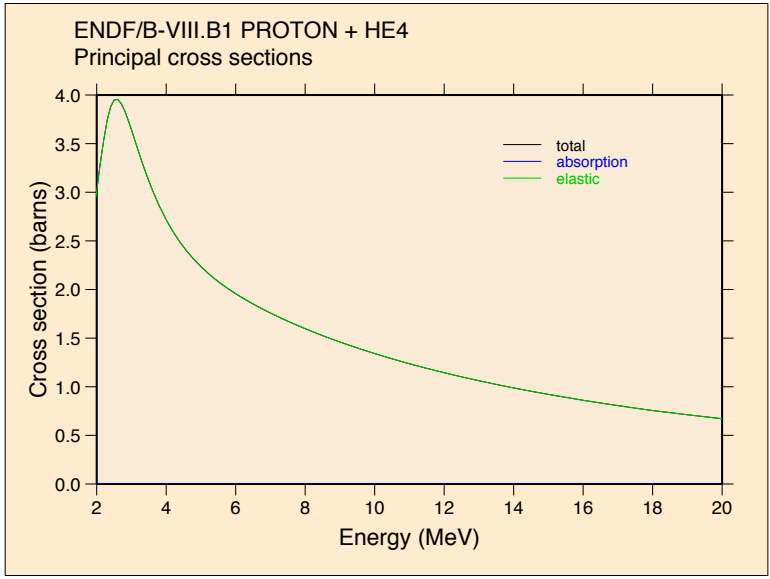

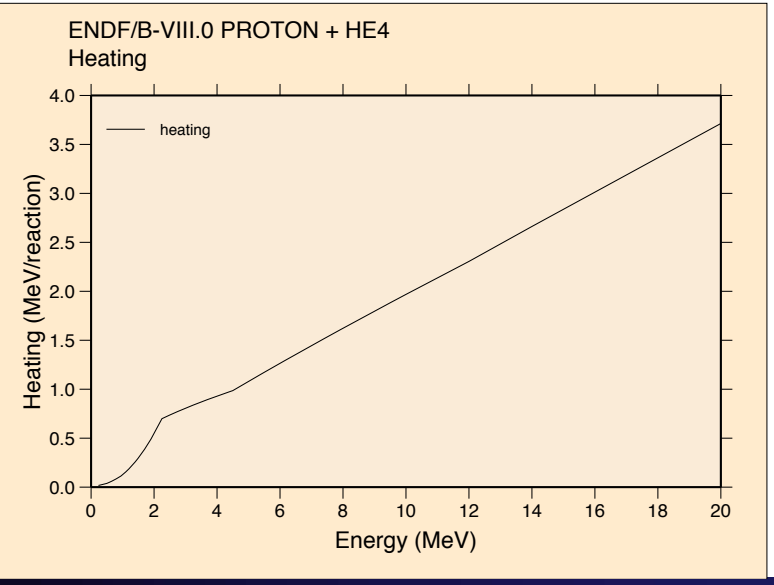

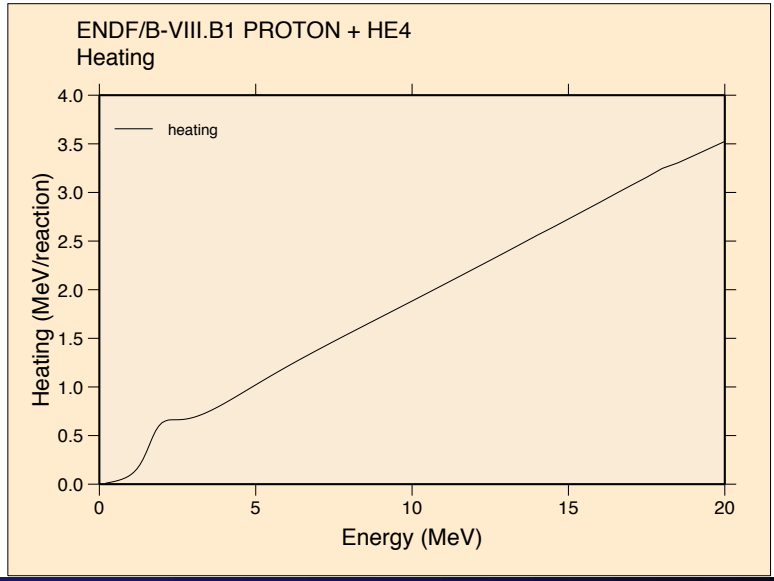

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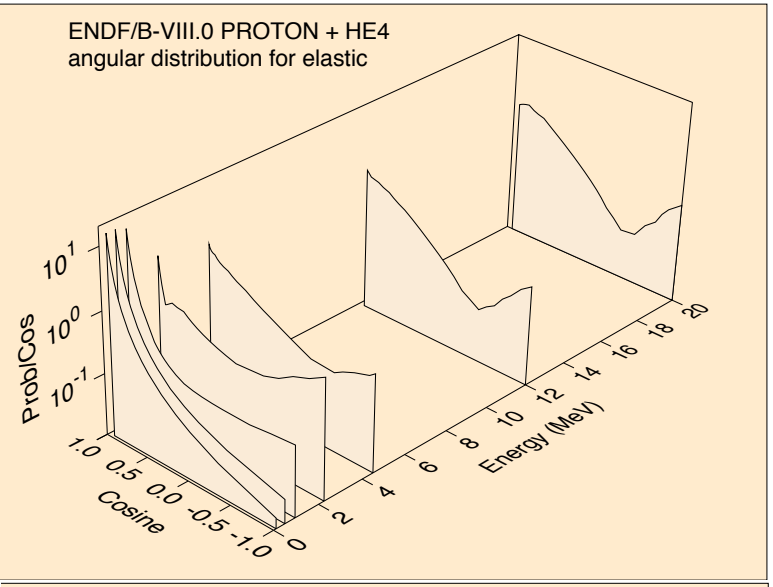

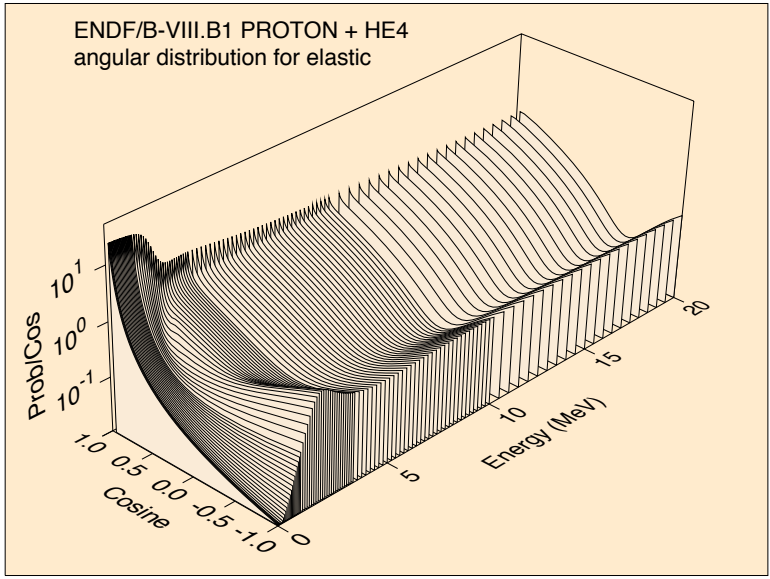

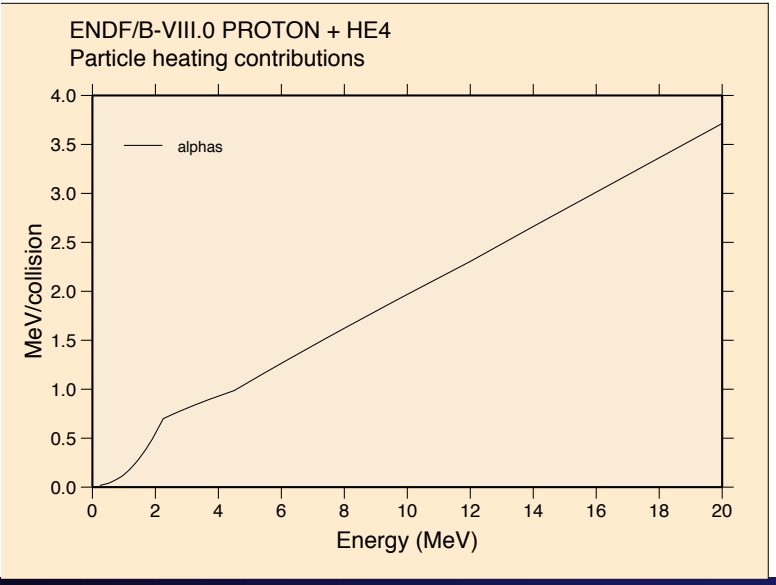

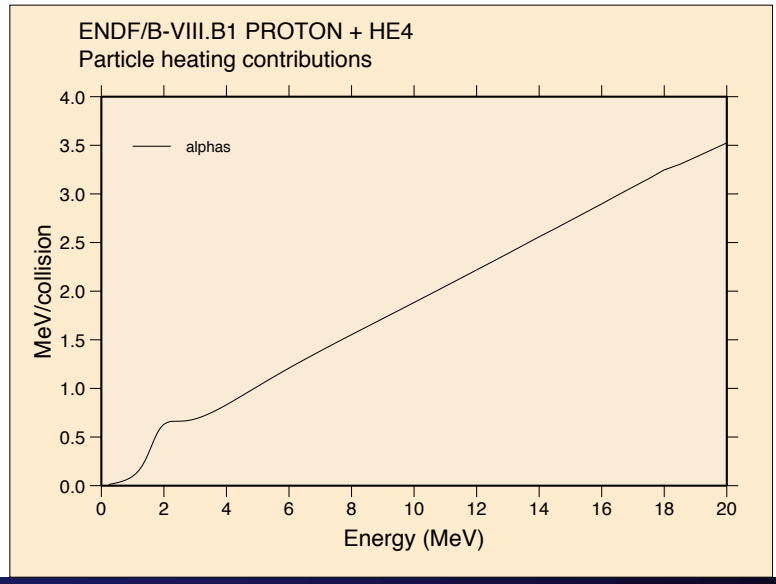

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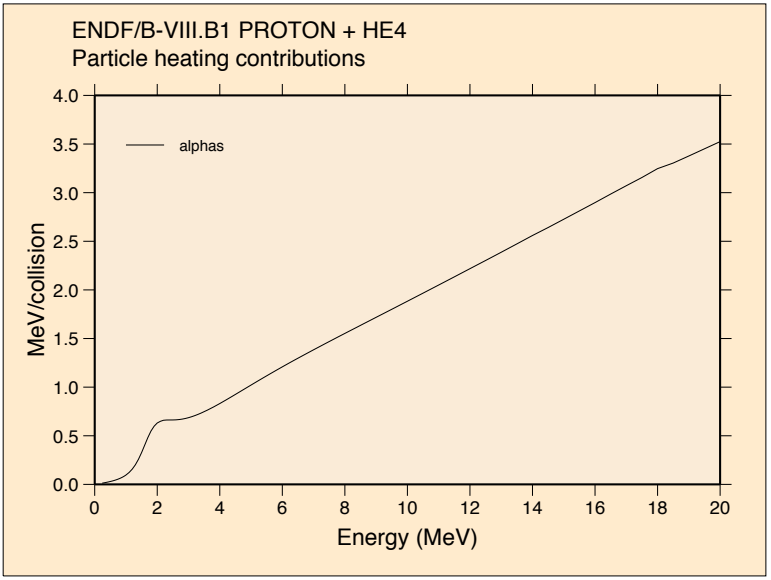

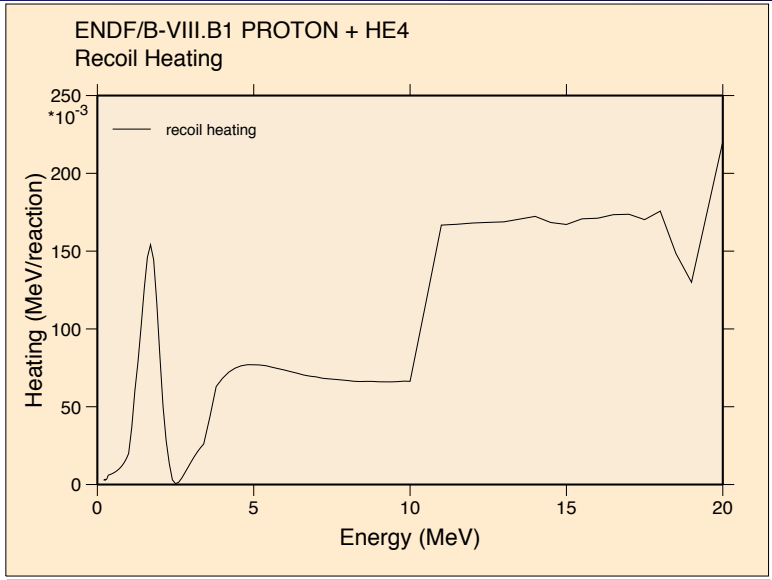

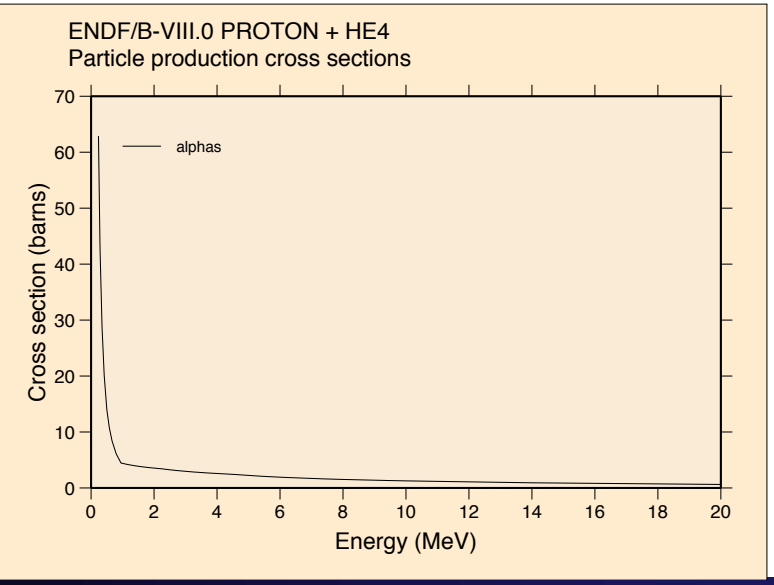

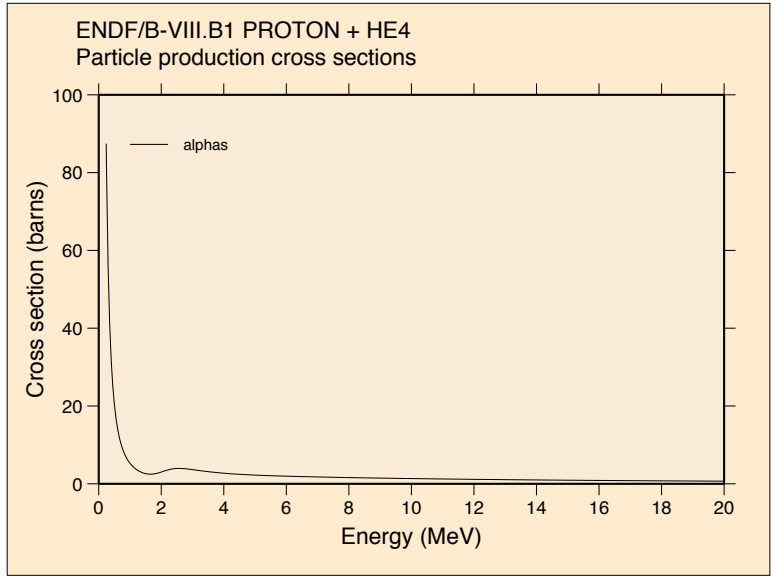

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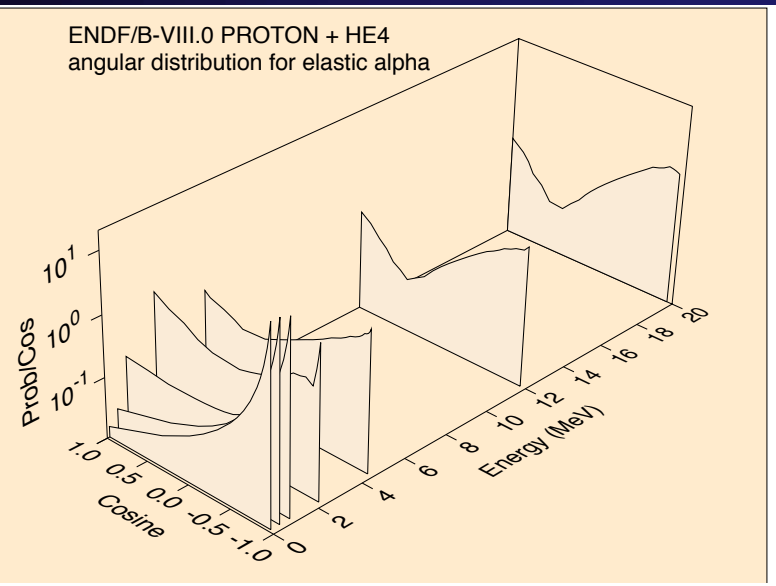

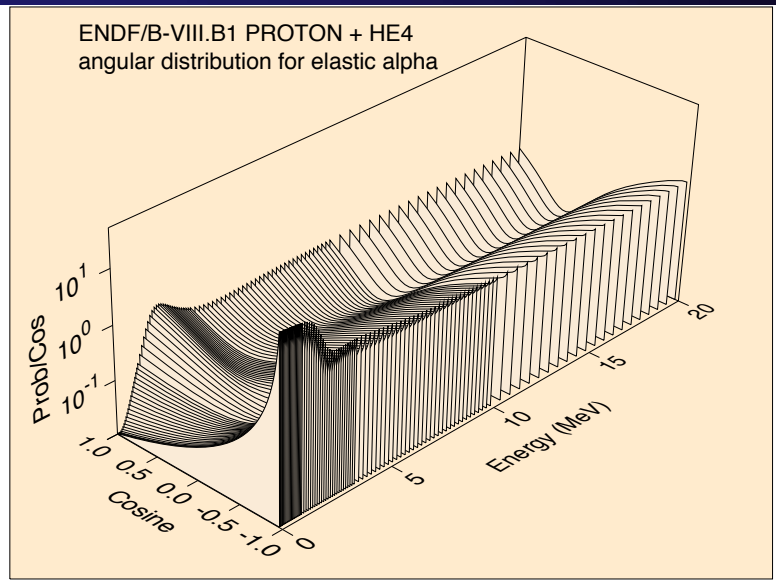

Status of existing LANL evaluations ENDF/B-VIII.0

Highlights

1. p+t, p+^{3}He, p+^{6,7}Li
2. d+d, d+t, d+^{3}He
3. t+t, t+^{6}Li
4. n+^{6}Li, n+^{12}C, n+^{13}C
5. ^{9}Be system
6. ^{15}N system
7. n+^{16}O

Existing LANL evaluations

A	System	Channels	Energy Range (MeV)
2	N-N	p+p; n+p, γ+d	0-40 0-40
3	N-d	p+d; n+d	0-4
4	^{4}H; ^{4}Li	n+t; p+^{3}He	0-20
	^{4}He	p+t; n+^{3}He; d+d	0-11; 0-10; 0-10
5	^{5}He	n+α; d+t; ^{5}He+γ	0-28; 0-10
	^{5}Li	p+α; d+^{3}He	0-24; 0-1.4

A	System (Channels)
6	^{6}He (^{5}He+n, t+t); ^{6}Li (d+^{4}He, t+^{3}He); ^{6}Be (^{5}Li+p, ^{3}He+^{3}He)
7	^{7}Li (t+^{4}He, n+^{6}Li); ^{7}Be (γ+^{7}Be, ^{3}He+^{4}He, p+^{6}Li)
8	^{8}Be (^{4}He+^{4}He, p+^{7}Li, n+^{7}Be, p+^{7}Li*, n+^{7}Be*, d+^{6}Li)
9	^{9}Be (^{8}Be+n, d+^{7}Li, t+^{6}Li); ^{9}B (γ+^{9}B, ^{8}Be+p, d+^{7}Be, ^{3}He+^{6}Li)
10	^{10}Be (n+^{9}Be, ^{6}He+α, ^{8}Be+nn, t+^{7}Li); ^{10}B (α+^{6}Li, p+^{9}Be, ^{3}He+^{7}Li)
11	^{11}B (α+^{7}Li, α+^{7}Li*, ^{8}Be+t, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)
12	^{12}C (^{8}Be+α, p+^{11}B)
13	^{13}C (n+^{12}C, n+^{12}C*)
14	^{14}C (n+^{13}C)
15	^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)
16	^{16}O (γ+^{16}O, α+^{12}C)
17	^{17}O (n+^{16}O, α+^{13}C)
18	^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)

Status of existing LANL evaluations ENDF/B-VIII.0

Proton induced

- **p-001_H_003.endf** **[T(p,x)Y]**
  - MF3(x-sec): 2(el), 50(n_0), 650(d_0) (<20 MeV)
  - MF6(E-ang): 2, 50, 600
- **p-002_He_003.endf** **[^{3}He(p,x)Y]**
  - MF3: 2(el), 50(n_0), 650(d_0) (<20 MeV)
  - MF6: 2, 50, 650
- **p-002_He_004.endf** **[^{4}He(p,x)Y]**
  - LLNL
- **p-003_Li_006.endf** **[^{6}Li(p,x)Y]**
  - MF3: 2 750 (^{3}He$_0$) (<2.5 MeV)
  - MF6: 2 750
- **p-003_Li_007.endf** **[^{7}Li(p,x)Y]**
  - LLNL

Status of existing LANL evaluations ENDF/B-VIII.0

Deuteron induced

- **d-001_H_002.endf** **[D(d,x)Y]**
  - MF3(x-sec): 2(el), 50(n0), 600(p0) (<10 MeV)
  - MF6(E-ang): 2, 50, 600 (<10 MeV)
- **d-001_H_003.endf** **[T(d,x)Y]**
  - MF3: 2 50(<40 MeV) 51 (<10 MeV)
  - MF6: 2 50 51 (same energies)
- **d-002_He_003.endf** **[^{3}He(d,x)Y]**
  - MF3: 2 600 (<14 MeV)
  - MF6: 2 600
- **d-002_He_004.endf** **[^{3}He(d,x)Y]**
  - MF3: 2 28 (<10 MeV)
  - MF6: 2
- **d-003_Li_006.endf** **[^{6}Li(d,x)Y]**
  - MF3: 2 50 600 800(a0) (<5 MeV)
  - MF6: 2 50 600 800
- **d-003_Li_007.endf** **[^{7}Li(d,x)Y]**
  - LLNL

Status of existing LANL evaluations ENDF/B-VIII.0

Triton/alpha induced

- **t-001_H_003.endf** **[T(t,x)Y]**
  - MF3: 2 16(2n) (<2.2 MeV Rmat/data; >2.2, <20 extrap)
  - MF6: 2 16
- **t-002_He_003.endf** **[^{3}He(t,x)Y]**
  - MF3: 2 28(np) 650(nd) (<3 MeV Rmat/data; >3, <20 extrap)
  - MF6: 2 28 650
- **t-002_He_004.endf** **[^{4}He(t,x)Y]**
  - LLNL
- **t-003_Li_006.endf** **[^{6}Li(t,x)Y]**
  - MF3: 2 22(nα) 650 (<4 MeV Rmat/data; >4, <20 MeV extrap)
  - MF6: 2 22 650
- **t-003_Li_007.endf** **[^{7}Li(t,x)Y]**
  - LLNL
- **a-002_He_004.endf** **[^{4}He(a,x)Y]**
  - MF6: 2 (<20 MeV)

Ongoing work

- **Commit existing charged-particle evaluations to ENDF git repos**
  - protons: ^{4}He, ^{7}Li
  - deuterons: ^{4}He, ^{7}Li
  - tritons: ^{4}He
  - ^{3}He's: ^{3}He, ^{4}He
  - alphas: ^{4}He
- **Ongoing evaluation work**
  - Spectra of all sorts
  - *Covariances*
  - Charged-particle production and induced reactions
  - n+^{9}Be, n+^{16}O (interest from NCSP)
  - NN up to 250 MeV (interest from IAEA/standards)
  - Lots of others...
- **Public release of EDA R-Matrix parameters**
  - `LRF=7, KRL=1` relativistic parametrization
- **Code modernization EDA5→EDA6**
  - data/exp'l IRF, likelihood (Bayes) fitting, integral exp interface, GNDS,...
  - Perhaps in 2020

Thank you!

Follow-on material

Status of existing LANL evaluations ENDF/B-VIII.0

Neutron induced

```
==> neutrons-VIII_0_owners.txt <==
 0 - N - 1 LANL        EVAL-APR16 HALE, PARIS                          25 1451
  1-H -  1 LANL        EVAL-JUL16 G.M.Hale                            125 1451
  1-H -  2 LANL        EVAL-FEB97 P.G.Young,G.M.Hale,M.B.Chadwick     128 1451
  1-H -  3 LANL        EVAL-NOV01 G.M.Hale                            131 1451
  2-He-  3 LANL        EVAL-MAY90 G.Hale,D.Dodder,P.Young             225 1451
  2-He-  4 LANL        EVAL-SEP10 Hale                                228 1451
  3-Li-  6 LANL        EVAL-JAN17 G.M. Hale                           325 1451
  3-Li-  7 LANL        EVAL-AUG88 P.G.Young                           328 1451
  4-Be-  7 LANL        EVAL-JUN16 I.Thompson, P.R.Page                419 1451
  4-Be-  9 LLNL,LANL   EVAL-OCT09 G.HALE,PERKINS ET AL,FRANKLE        425 1451
  5-B - 10 LANL        EVAL-FEB17 G.M.Hale                            525 1451
  5-B - 11 LANL        EVAL-MAY89 P.G.Young                           528 1451
  6-C - 12 LANL,ORNL   EVAL-AUG15 G.M. Hale, P.G. Young, C.Y. Fu      625 1451
  6-C - 13 LANL,       EVAL-AUG15 G.M. Hale, M.W. Paris               628 1451
  7-N - 14 LANL        EVAL-JUN97 M.B.Chadwick,P.G.Young              725 1451
  7-N - 15 LANL        EVAL-SEP83 E.Arthur,P.Young,G.Hale             728 1451
  8-O - 16 LANL        EVAL-DEC16 Hale,Paris,Young,Chadwick           825 1451
```

ENDF/B-VIII.0 evaluation custodians

```
==> alphas-VIII_0_owners.txt <==
  2-He-  4 LLNL       EVAL-DEC99 R.M.White,D.A.Resler,S.I.Warshaw  228 1451
==> deuterons-VIII_0_owners.txt <==
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  1-H -  3 LANL       EVAL-JAN95 G.M.HALE  AND M.DROSG             131 1451
  2-He-  3 LANL       EVAL-FEB01 G.M.HALE                          225 1451
  3-Li-  6 LANL       EVAL-JUN04 P.R.PAGE                          325 1451
  3-Li-  7 LLNL       EVAL-NOV10 P. Navratil, D. A. Brown          328 1451
==> helium3s-VIII_0_owners.txt <==
  2-He-  3 LLNL       EVAL-NOV10 P.Navratil, D.Brown, G.Hale       225 1451
  2-He-  4 LLNL       EVAL-DEC99 R.M.White,D.A.Resler,S.I.Warshaw  228 1451
  3-Li-  6 LANL       EVAL-NOV02 G.M.HALE                          325 1451
==> neutrons-VIII_0_owners.txt <==
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  1-H -  1 LANL       EVAL-JUL16 G.M.Hale                          125 1451
  1-H -  2 LANL       EVAL-FEB97 P.G.Young,G.M.Hale,M.B.Chadwick   128 1451
  1-H -  3 LANL       EVAL-NOV01 G.M.Hale                          131 1451
  2-He-  3 LANL       EVAL-MAY90 G.Hale,D.Dodder,P.Young           225 1451
  2-He-  4 LANL       EVAL-SEP10 Hale                              228 1451
  3-Li-  6 LANL       EVAL-JAN17 G.M. Hale                         325 1451
  3-Li-  7 LANL       EVAL-AUG88 P.G.Young                         328 1451
  4-Be-  7 LANL       EVAL-JUN16 I.Thompson, P.R.Page              419 1451
  4-Be-  9 LLNL,LANL  EVAL-OCT09 G.HALE,PERKINS ET AL,FRANKLE      425 1451
  5-B - 10 LANL       EVAL-FEB17 G.M.Hale                          525 1451
  5-B - 11 LANL       EVAL-MAY89 P.G.Young                         528 1451
  6-C - 12 LANL,ORNL  EVAL-AUG15 G.M. Hale, P.G. Young, C.Y. Fu    625 1451
  6-C - 13 LANL,      EVAL-AUG15 G.M. Hale, M.W. Paris             628 1451
  7-N - 14 LANL       EVAL-JUN97 M.B.Chadwick,P.G.Young            725 1451
  7-N - 15 LANL       EVAL-SEP83 E.Arthur,P.Young,G.Hale           728 1451
  8-O - 16 LANL       EVAL-DEC16 Hale,Paris,Young,Chadwick         825 1451
```
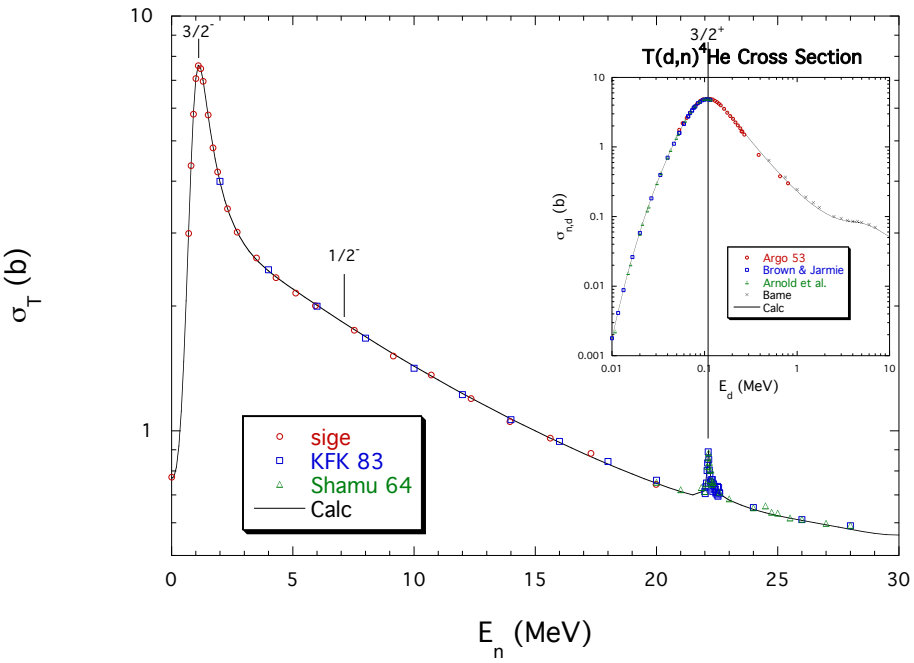

ENDF/B-VIII.0 evaluation custodians (cont.)

```
==> protons-VIII_0_owners.txt <==
  1-H -  1 LANL       EVAL-FEB98 G.HALE                              125 1451
  1-H -  2 LANL       EVAL-FEB97 P.G.YOUNG,G.M.HALE,M.B.CHADWICK     128 1451
  1-H -  3 LANL       EVAL-SEP01 G. M. HALE                          131 1451
  2-He-  3 LANL       EVAL-OCT83 G.HALE                              225 1451
  2-He-  4 LLNL       EVAL-DEC99 R.M.White,D.A.Resler,S.I.Warshaw    228 1451
  3-Li-  6 LANL       EVAL-AUG01  G.M.HALE                           325 1451
  3-Li-  7 LLNL       EVAL-SEP10 P. Navratil, D.A. Brown             328 1451
  4-Be-  9 LANL       EVAL-NOV88 P.G.Young, E.D.Arthur               425 1451
  5-B - 10 LANL       EVAL-AUG05   P.R.PAGE                          525 1451
  6-C - 12 LANL       EVAL-JUN96 M.B.CHADWICK AND P.G.YOUNG          625 1451
  6-C - 13 LANL       EVAL-DEC04  P.R.PAGE                           628 1451
  7-N - 14 LANL       EVAL-AUG97 M.B.CHADWICK & P.G.YOUNG            725 1451
  8-O - 16 LANL       EVAL-JUN96 M.B.CHADWICK AND P.G.YOUNG          825 1451
==> tritons-VIII_0_owners.txt <==
  1-H -  3 LANL       EVAL-FEB01 G.M.HALE                            131 1451
  2-He-  3 LANL       EVAL-AUG01 G.M.HALE                            225 1451
  2-He-  4 LLNL       EVAL-DEC99 R.M.White,D.A.Resler,S.I.Warshaw    228 1451
  3-Li-  6 LANL       EVAL-SEP01 G.M.HALE                            325 1451
  3-Li-  7 LLNL       EVAL-JUN16 I.Thompson, P.Navratil, D.Brown     328 1451
```

T(d,n)α evaluation (I)

- **Simultaneously fits all known low-E data**
  - neutron & charged-particle channels
  - polarization (distinguishes partial waves, etc.)
- **High-fidelity X^2 ~ 1.5 below 10 MeV**
- **All resonances/partial waves included**
- **EDA also provides covariance matrices**

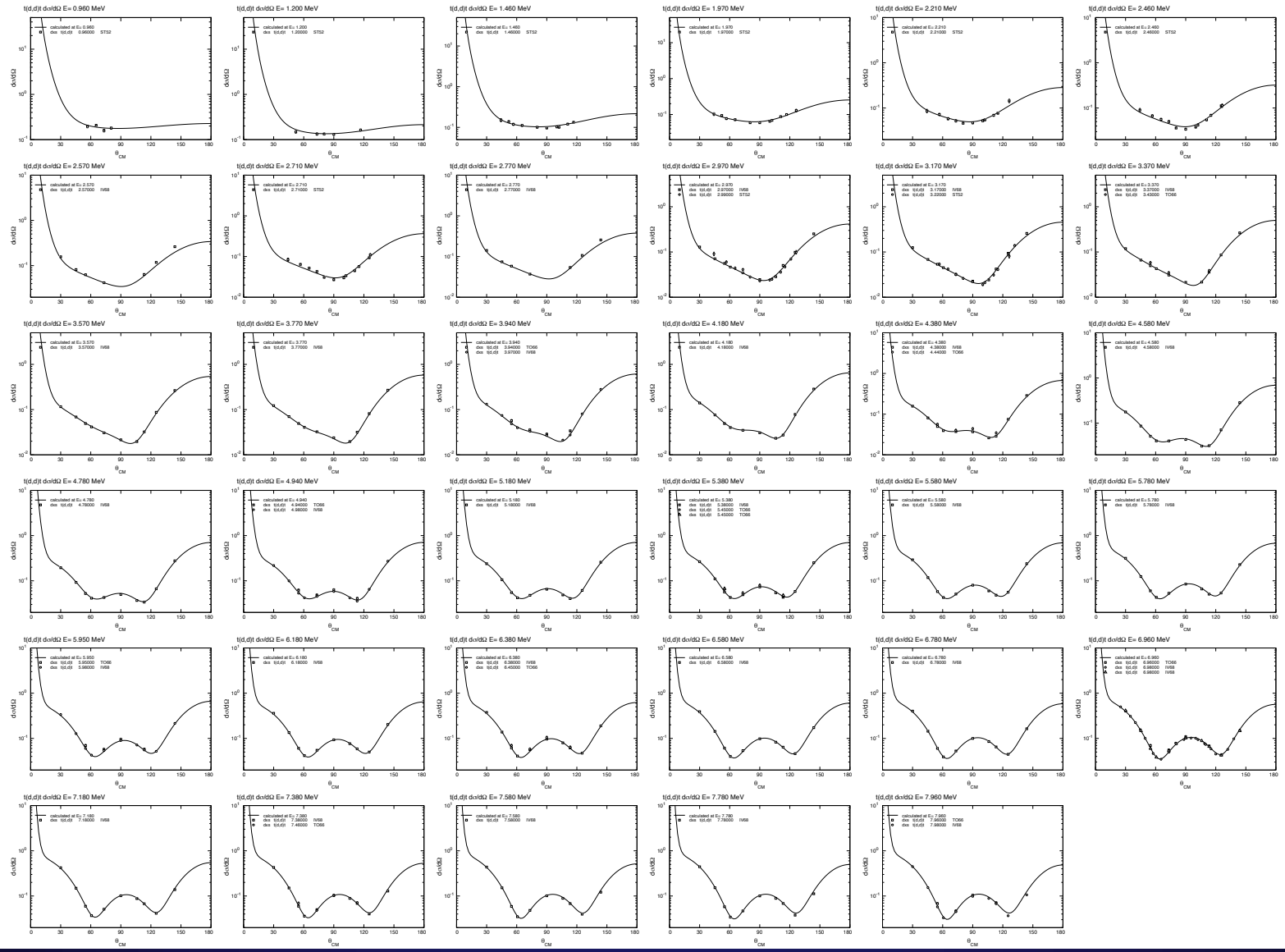


channel	a_c (fm)	l_{max}
n+^{4}He	3.0	5
γ+^{5}He	60	1
d+^{3}H	5.1	5
n+^{4}He*	5.0	1

Reaction	Energies (MeV)	# data points	# data types
^{4}He(n,n)^{4}He	E_n = 0 – 40	817	2
^{3}H(d,d)^{3}H	E_d = 0 – 8.6	700	6
^{3}H(d,n)^{4}He	E_d = 0 – 30	1185	14
^{3}H(d,γ)^{5}He	E_d = 0 – 8.6	17	2
^{3}H(d,n)^{4}He*	E_d = 4.8 – 8.3	10	1
total		2729	25

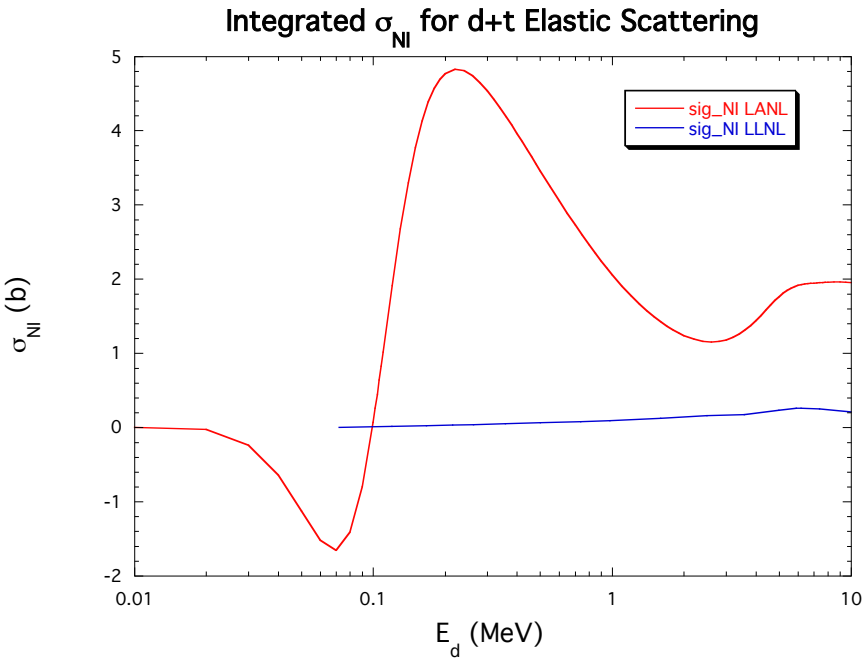
T(d,n)α evaluation (II)

Angular distributions T(d,el)



T(d,n)α evaluation (II)

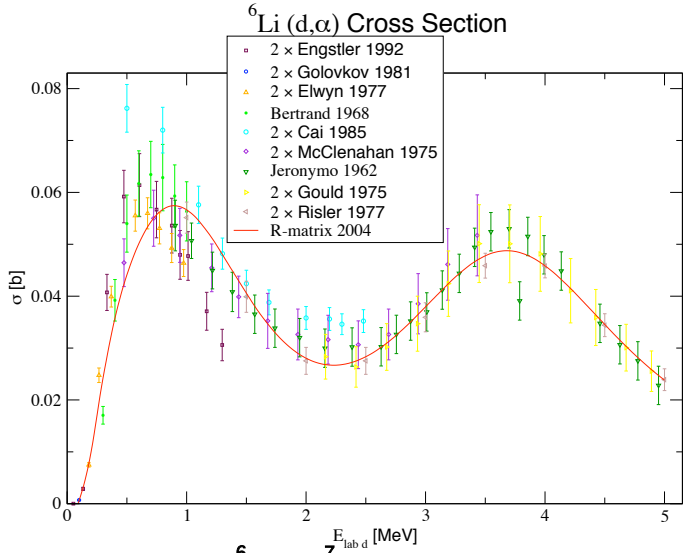
σ_{NI} T(d,el) nuclear plus interference

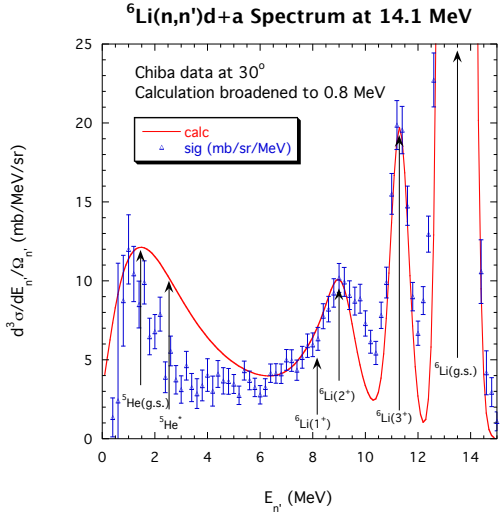


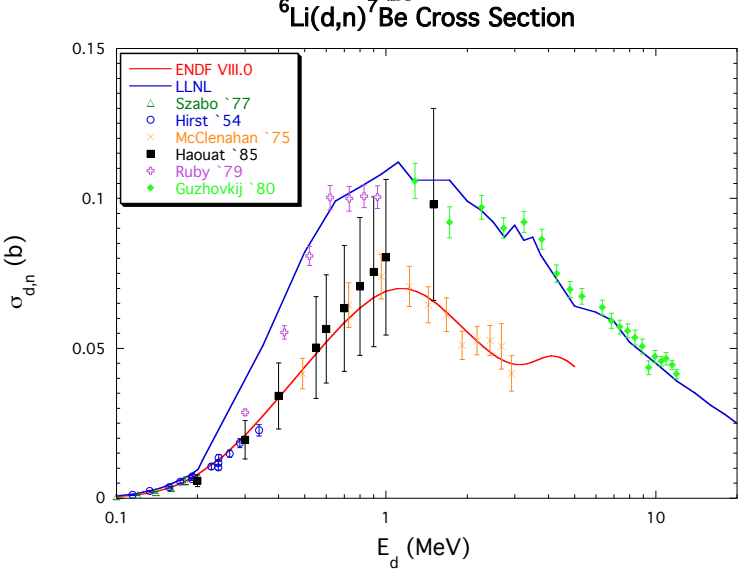
- **Nuclear + interference cross section**
  - requires multichannel fit
  - strong energy dependence
  - not necessarily > 0

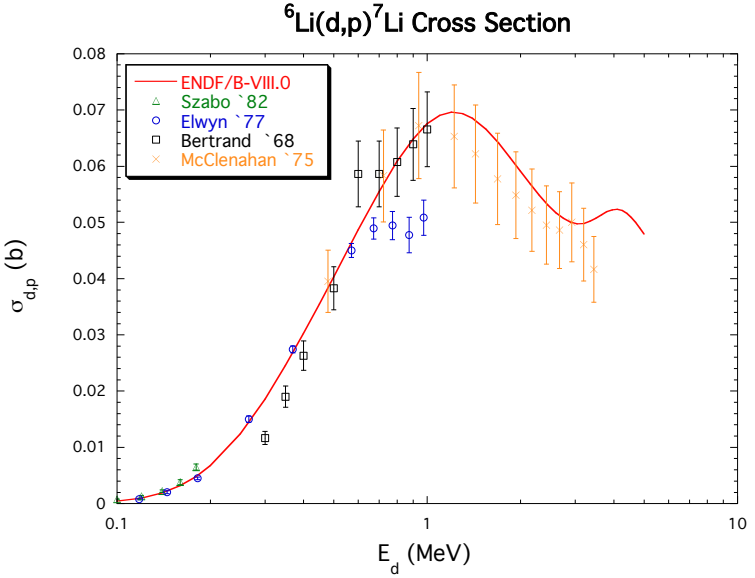
^{6}Li

deuterons, neutrons









Uncertainties from chi-squared minimization

$$\chi^2_{\mathrm{EDA}} = \sum_i \left[\frac{nX_i(\mathbf{p}) - R_i}{\Delta R_i}\right]^2 + \left[\frac{nS-1}{\Delta S/S}\right]^2$$

$$\begin{cases} R_i,\ \Delta R_i = \text{relative measurement, uncertainty} \\ S,\ \Delta S = \text{experimental scale, uncertainty} \\ X_i(\mathbf{p}) = \text{observable calc. from res. pars. } \mathbf{p} \\ n = \text{normalization parameter} \end{cases}$$

Near a minimum of the chi-squared function at $\mathbf{p} = \mathbf{p}_0$:

$$\begin{aligned} \chi^2(\mathbf{p}) &= \chi^2_0 + (\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0) \\ &= \chi^2_0 + \Delta\chi^2. \end{aligned}$$

$$\begin{cases} \chi^2_0 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

Conventions:

1) previous: $\Delta\chi^2 = 1 \implies$ Very small uncertainties $\delta p_i = (C^0_{ii})^{1/2} \sim \mathcal{O}(N_p^{-1/2})$

2) improved: $\Delta\chi^2 = \frac{1}{2}\Delta\mathbf{p}^{\mathrm{T}}\mathbf{G}_0\Delta\mathbf{p} \le \Delta\chi^2_{\max}$,

$$P(\Delta\chi^2|k) = \left[2^{\frac{k}{2}}\Gamma(\tfrac{k}{2})\right]^{-1}\int_0^{\Delta\chi^2_{\max}} t^{\frac{k}{2}-1}e^{-\frac{t}{2}}dt = \mathrm{CL}\ (\text{e.g.} \sim 0.68 \text{ for 1-}\sigma),\ 0.95 \text{ for 2-}\sigma, \text{etc.}$$

$$\Delta\chi^2_{\max} \approx k = \left\langle \Delta\chi^2 \right\rangle.$$

$$\delta p_i \sim (N_p C^0_{ii})^{1/2}$$

Covariance

The parameter covariance matrix is $\mathbf{C}_0 = 2\mathbf{G}_0^{-1}$, and so first-order error propagation gives for the cross-section covariances

$$\chi^2(\mathbf{p}) = \chi_0^2 + (\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0)$$
$$= \chi_0^2 + \Delta\chi^2.$$

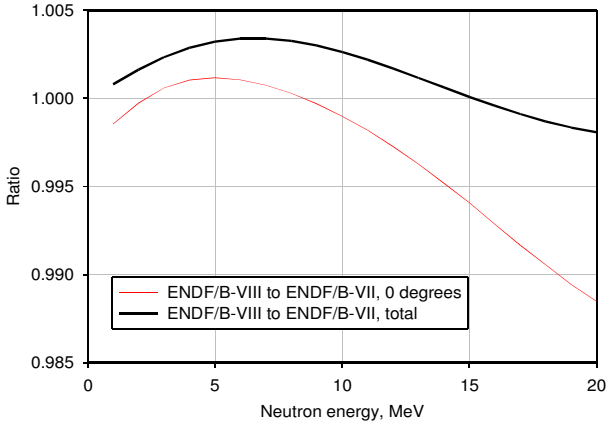
$$\begin{cases} \chi_0^2 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\Big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\Big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

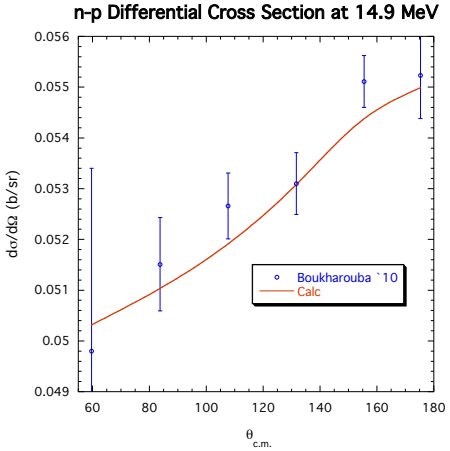
$$\mathrm{cov}[\sigma_{\mathrm{i}}(E)\sigma_j(E')] = \left[\nabla_{\mathbf{p}}\sigma_{\mathrm{i}}(E)\right]^{\mathrm{T}}\mathbf{C}_0\left[\nabla_{\mathbf{p}}\sigma_{\mathrm{j}}(E')\right]\Big|_{\mathbf{p}=\mathbf{p}_0}$$
$$= \Delta\sigma_{\mathrm{i}}(E)\Delta\sigma_{\mathrm{j}}(E')\rho_{ij}(E,E').$$

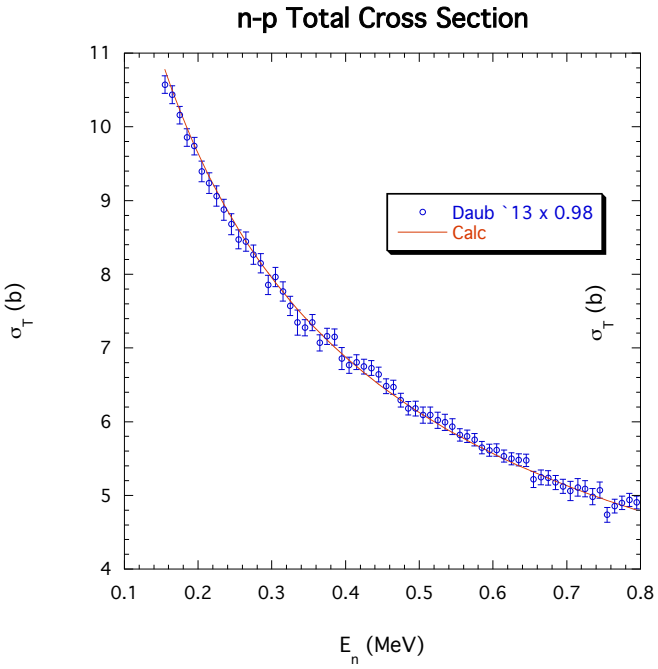
observable uncertainties

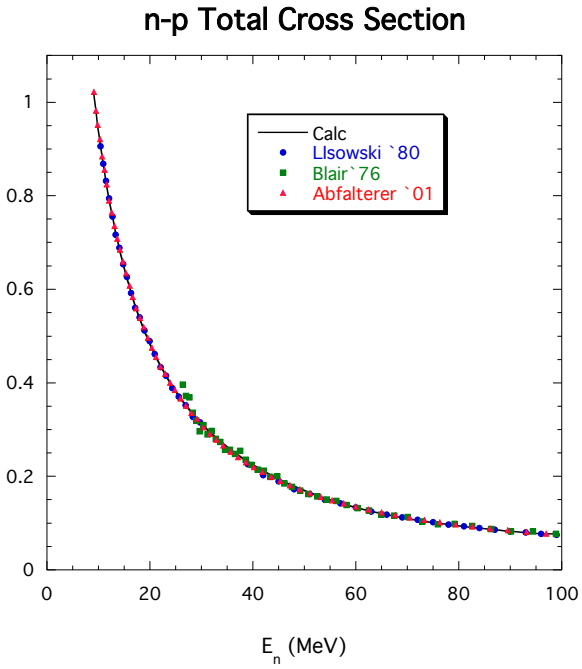
correlation coefficient

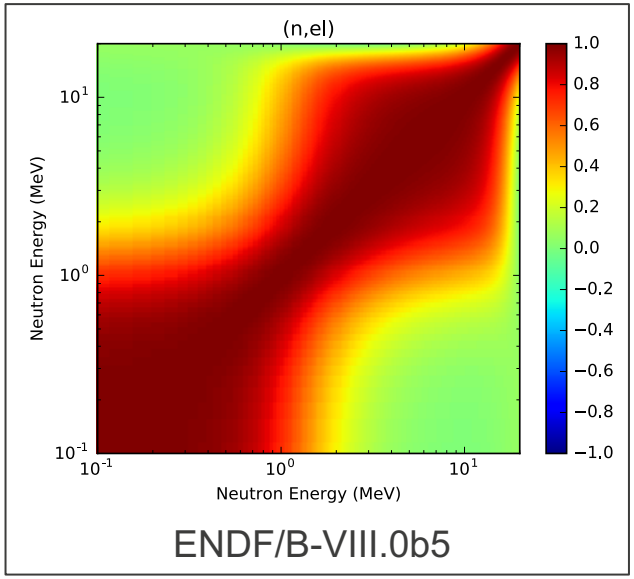
Evaluation 1: n-001_H_001











Partitions:

$pp(\ell \leq 3); np(\ell \leq 3);$
$\gamma d(\ell \leq 1); nn(\ell \leq 3)$

36 channels $(J^\pi LS)$

$\chi^2/\text{dof} \simeq 0.9$

Evaluation 2: n-003_Li_006

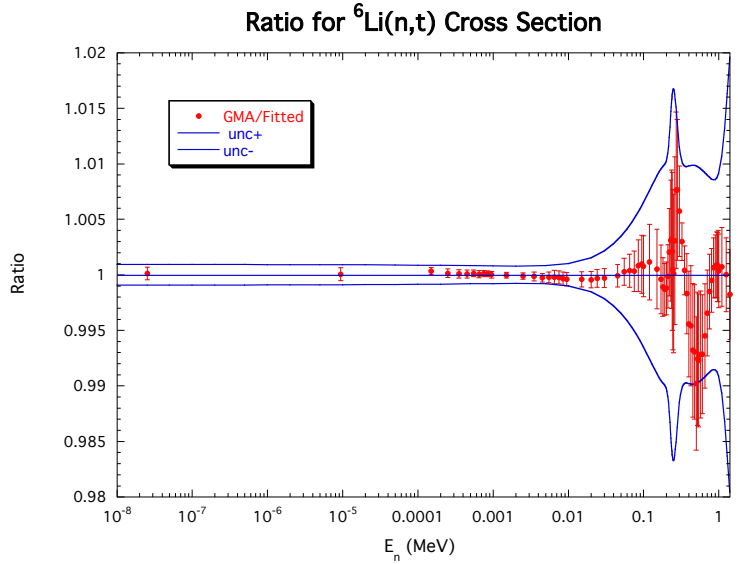
Partitions :

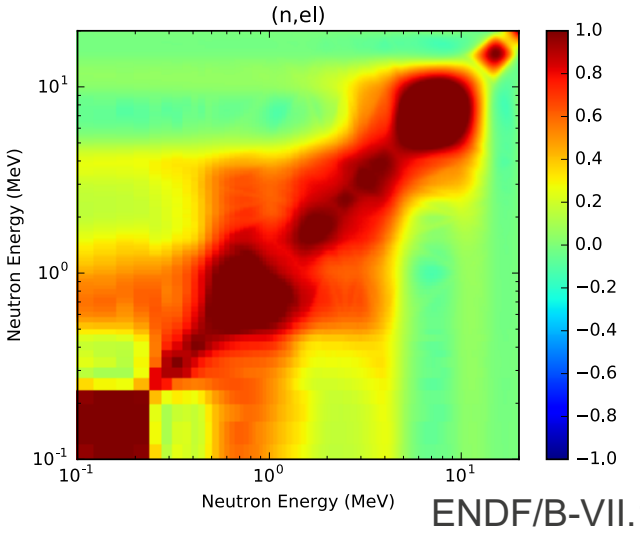
$t^4\mathrm{He}(\ell \leq 5); n^6\mathrm{Li}(\ell \leq 3);$

$n^6\mathrm{Li}^*(\ell \leq 1); d^5\mathrm{He}(\ell = 0)$

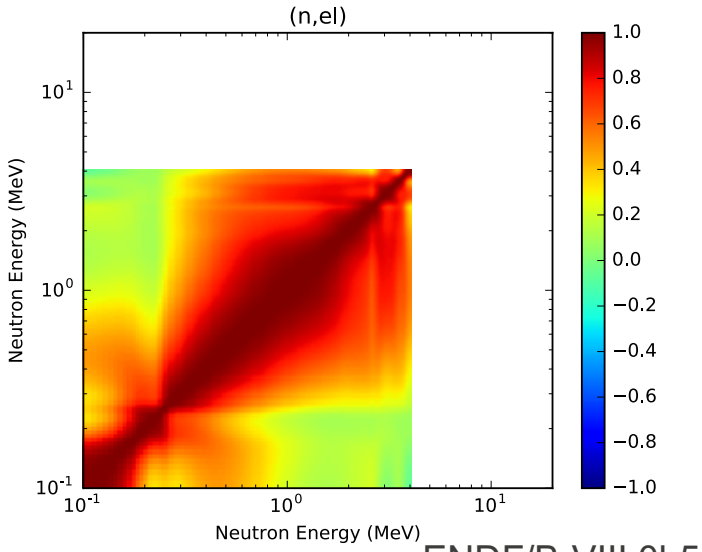
41 channels $(J^\pi LS)$

$\chi^2/\mathrm{dof} = 1.36$

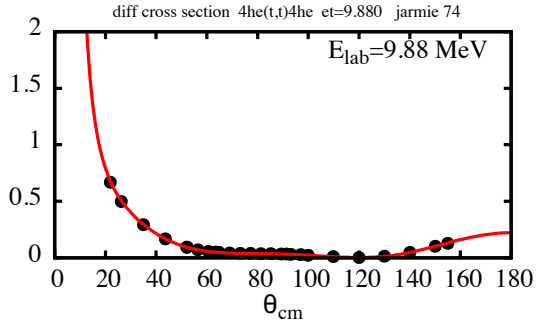


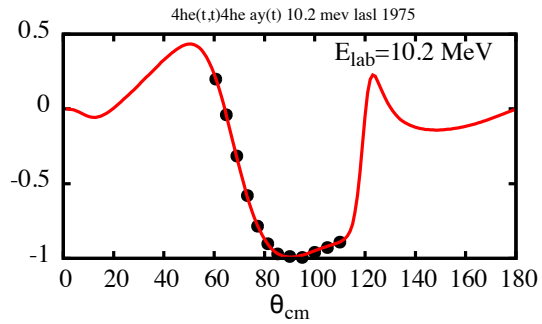


ENDF/B-VII.1

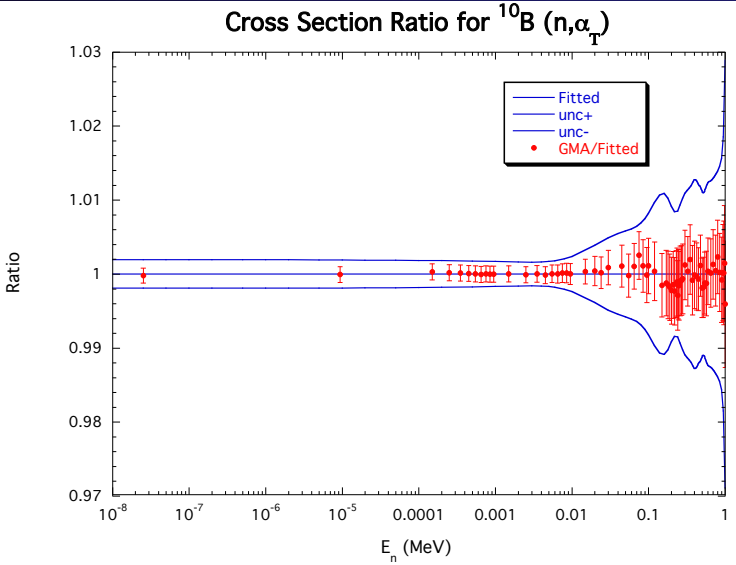


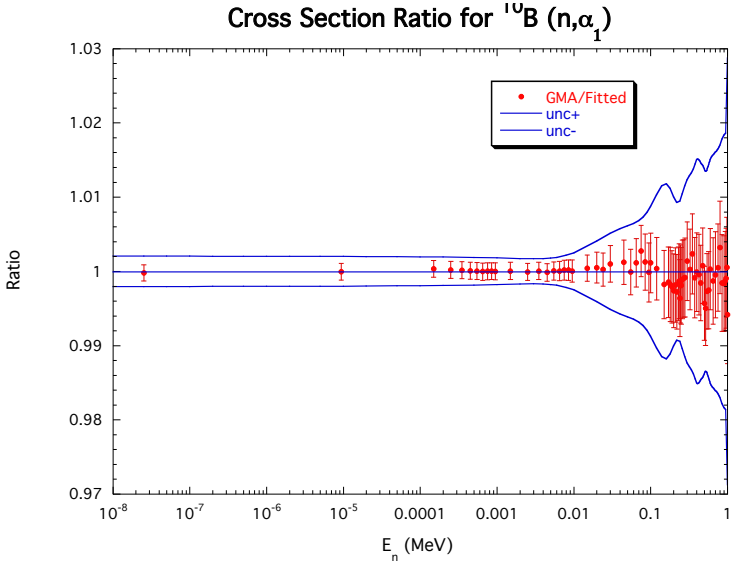
ENDF/B-VIII.0b5





Evaluation 3: n-005_B_010





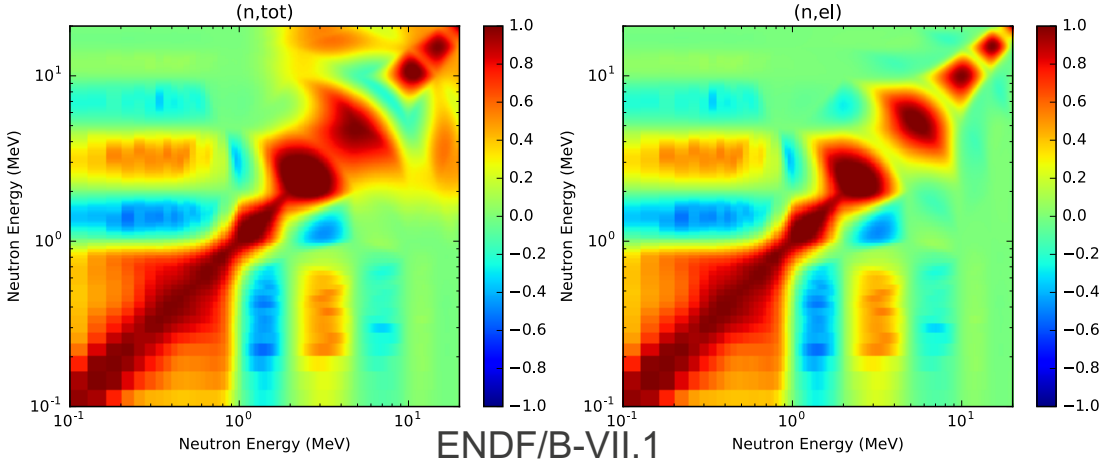
Partitions :

$n^{10}\mathrm{B}(\ell \leq 1); \alpha^{7}\mathrm{Li}(\ell \leq 3);$

$\alpha^{7}\mathrm{Li}^{*}(\ell \leq 1); t^{8}\mathrm{Be}(\ell \leq 2)$

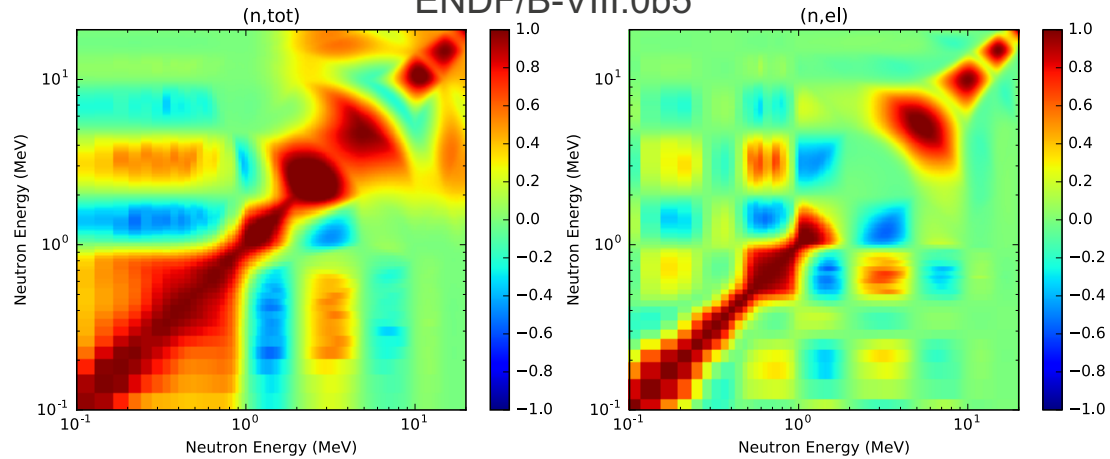
32 channels $(J^{\pi} LS)$

$\chi^2/\mathrm{dof} = 1.14$

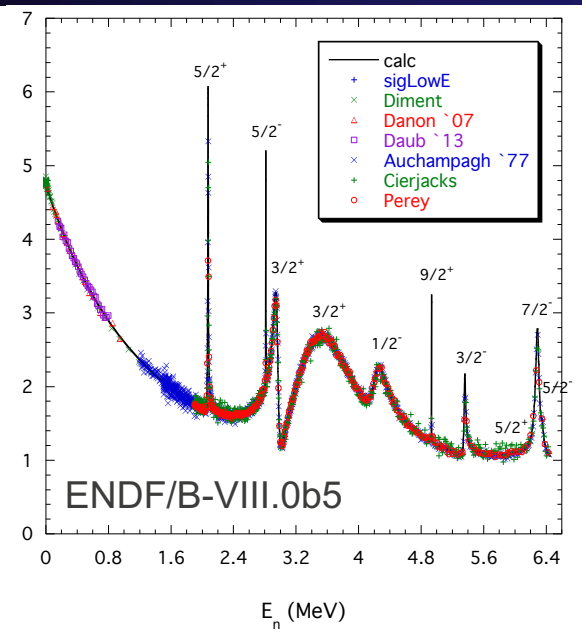


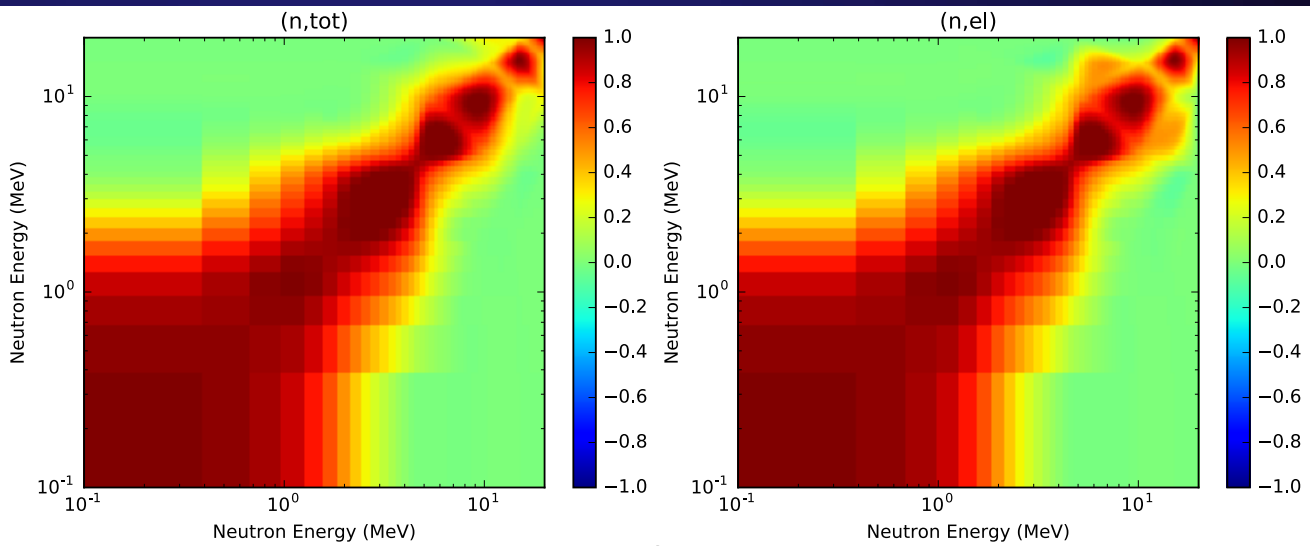
ENDF/B-VII.1

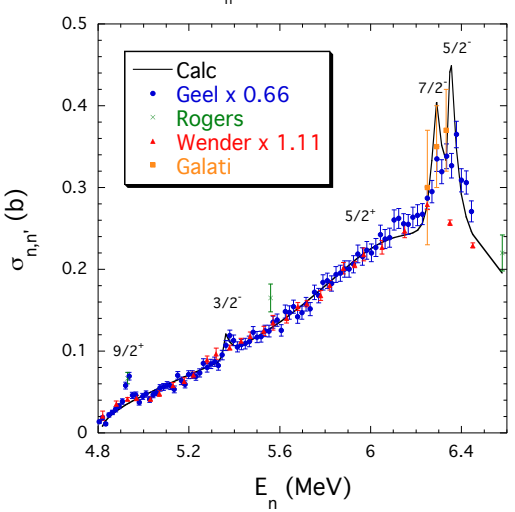
ENDF/B-VIII.0b5



Evaluation 4: n-006_C_012



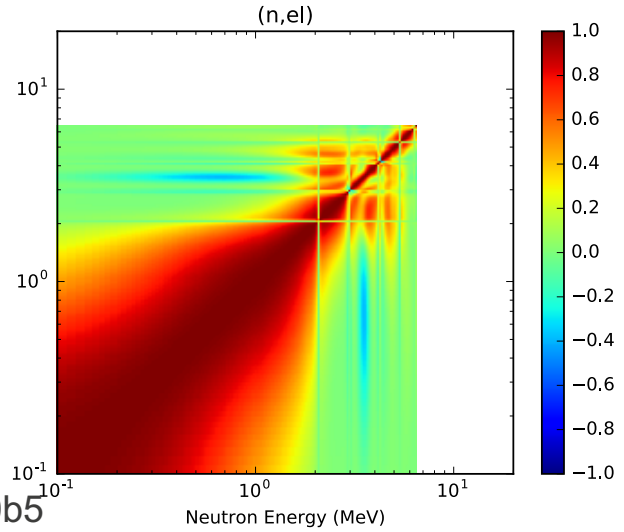




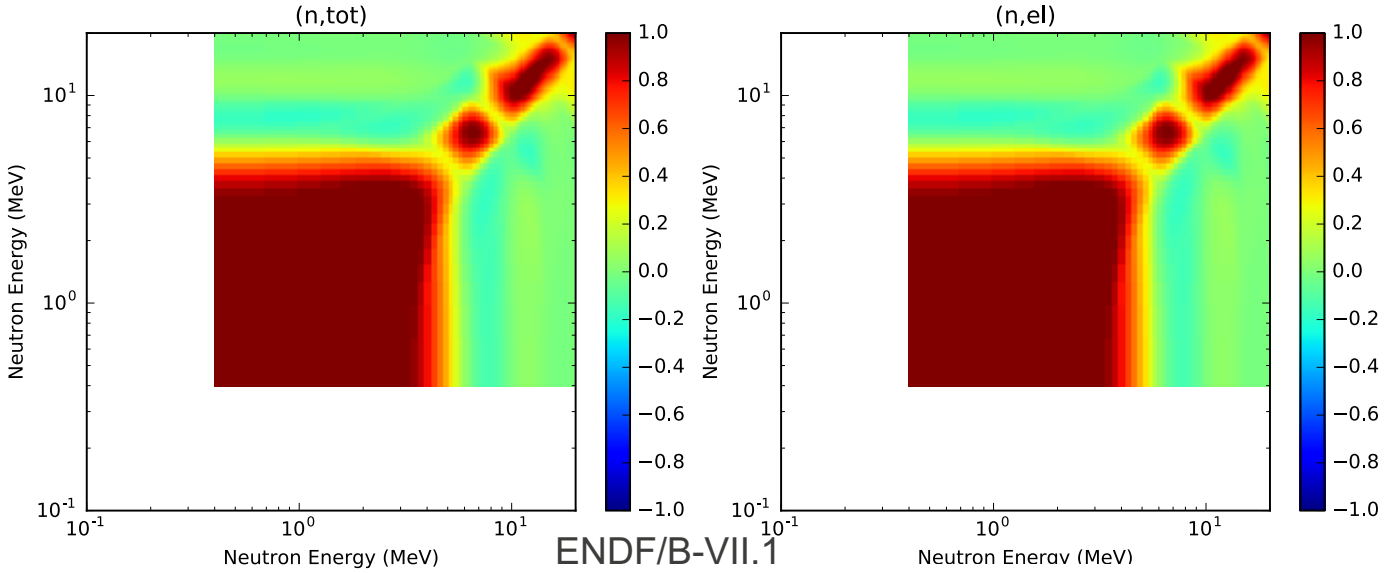
channel	a_c (fm)	l_{max}
n+^{12}C(0$^+$)	4.6	4
n+^{12}C*(2$^+$)	5.0	1
γ+^{13}C	50	1

Reaction	Energies (MeV)	# data points	Data types
^{12}C(n,n)^{12}C	E_n = 0 – 6.45	6940	σ_T, $\sigma(\theta)$, $A_n(\theta)$
^{12}C(n,n')^{12}C*	E_n = 5.3 – 6.45	443	σ_{int}, $\sigma(\theta)$
^{12}C(n,γ)^{13}C	E_n = 0 – 0.199	7	σ_{int}
total	4994	7390	5

χ^2 per degree of freedom = 1.54



Evaluation 5: n-008_O_016

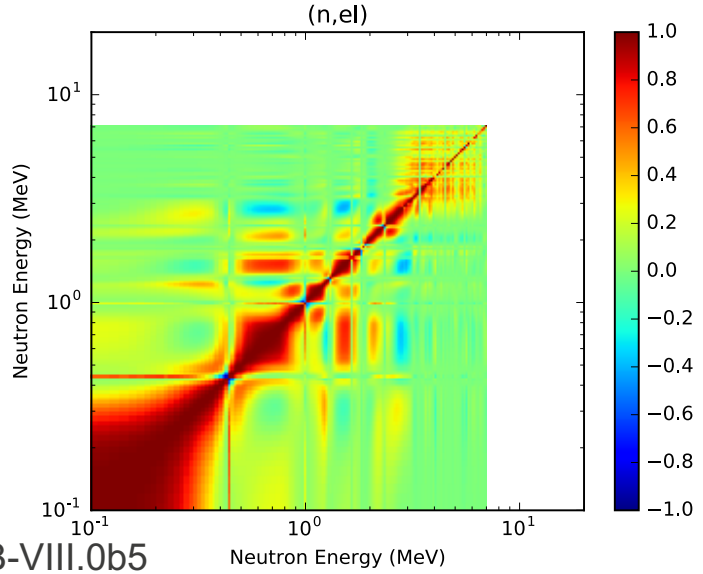


ENDF/B-VII.1

channel	a_c (fm)	l_{max}
n+^{16}O	4.4	4
α+^{13}C	5.4	5

Reaction	Energies (MeV)	# data points	Data types
^{16}O(n,n)^{16}O	E_n = 0 – 7	2540	σ_T, $\sigma(\theta)$, $P_n(\theta)$
^{16}O(n,α)^{13}C	E_n = 2.35 – 5	672	σ_{int}, $\sigma(\theta)$, $A_n(\theta)$
^{13}C(α,n)^{16}O	E_α = 0 – 5.4	870	σ_{int}
^{13}C(α,α)^{13}C	E_α = 2 – 5.7	1168	$\sigma(\theta)$
total		5250	8

χ^2 per degree of freedom = 1.68



ENDF/B-VIII.0b5