Los Alamos NATIONAL LABORATORY

Fusion-Relevant Light Element Nuclear Data Evaluations

Workshop for Applied Nuclear Data Activities (WANDA 2024)
Neutronics Session

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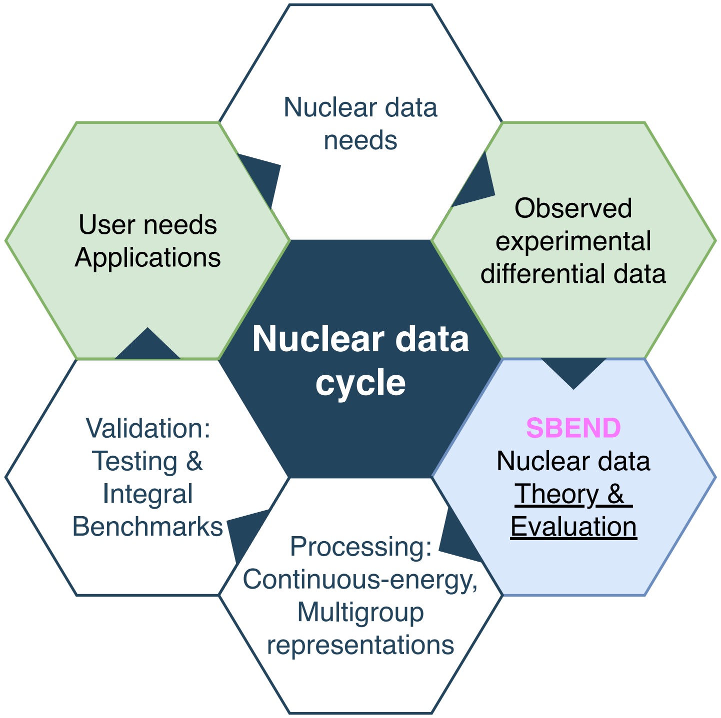
2024-02-26

LA-UR-24-21727

Outline

- What we do: R-matrix evaluation
- Evaluations
- Data generation/dissemination



Context

- Cross section evaluation working group (CSEWG)
  - Public Reusable (PuRe) research data
- Nuclear Data Interagency Working Group
  - SBEND Project
- Office of Science & Technology Programs (OSTP)
  - *Nuclear Data for Fusion Roundtable* (May 2023 meeting; Bahran's talk this AM)

Evaluation pipeline

How we do an R-matrix evaluation

Observation

- ***Single*** experiment observations of yield
- Unpolarized: $\sigma_{tot}, \sigma, \sigma(\theta)$
- Polarization: $P_n(E,\theta), A_y(E,\theta), K_x^{x'}, \ldots$

e.g. $\sigma(^{16}\mathrm{O}(n,n)^{16}\mathrm{O})$, $P_n(^{13}C(\alpha,\vec{n})^{16}O)$

→

Compilation

- Combination of single-experiment ***differential*** data (EXFOR/CSISRS)
- ***Compound-system*** data deck

e.g.: $^{17}\mathcal{O} = {}^{16}\mathrm{O}(n,n_i) + {}^{13}\mathrm{C}(\alpha,\alpha) + {}^{13}\mathrm{C}(\alpha,n_i) + {}^{16}\mathrm{O}(n,\alpha) + \cdots$

RULE: Include ***all*** data

→

Evaluation

- Determination of initial parameters $(E_\lambda, \gamma_{\lambda,c})$ from known/guessed resonance structure (ENSDF, TUNL-NDEP)
- Optimization of $\chi^2 = \sum_{\text{expt's}} \chi^2_{\text{expt}}$

→

Reaction Data

- Energy, angle, energy-angle dependent data formatting
- Formats: ENDF-6, GNDS, *etc.*

Structure & Decay Data

- Resonance properties: $E_j, \Gamma_{\text{tot,j}}, \Gamma_{j,c}, C_{j,c}$
- Formats: RIPL, ENSDF, ANR

`CODE implementation`

1. **`EDAf90`** code handles all types of data [*EXFOR/CSISRS; publications; priv. comm.*]
   - total, integrated, diff'l, unpolarized, ***polarized***; photon, neutron- and CP-induced: (γ,X), (n,X), (p,X), (d,X), (t,X),...
2. **`EDAf90`** handles all the compound system (here: **^{10}Be**) data ***simultaneously***
3. Optimization over parameters simultaneously fits all the data with the same parameters
4. **`EDAf90`** → ENDF-6 formatted ENDF/B libraries for processing to CE & MG libraries
5. Testing & evaluation by hand; future: automate

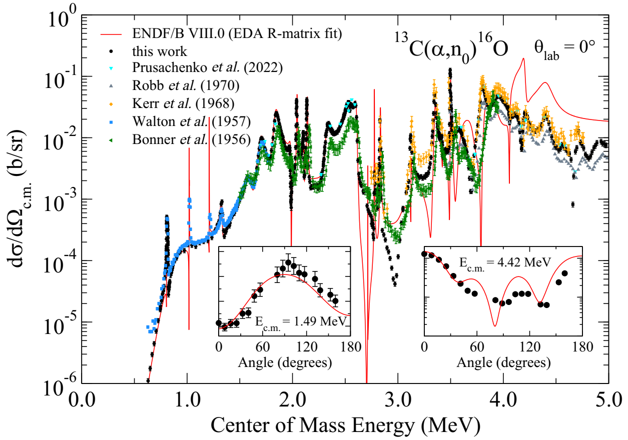
Evaluation of nuclear data

What, why, how, when?

Applications (*i.e.*, codes) need information that's:

- Accurate (consistent with observed data)
- Precise (uncertainties quantified)
- Comprehensive (energies, data types)
- Compact
- Format agnostic
- Smooth (differentiable)

We need to put these:



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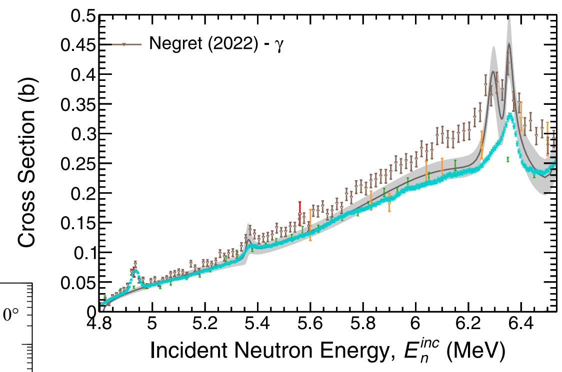

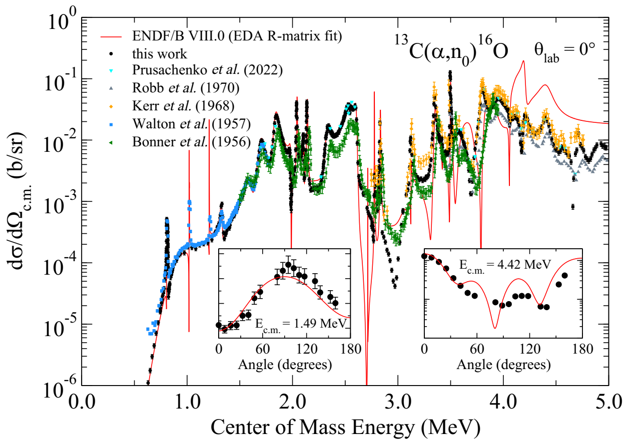

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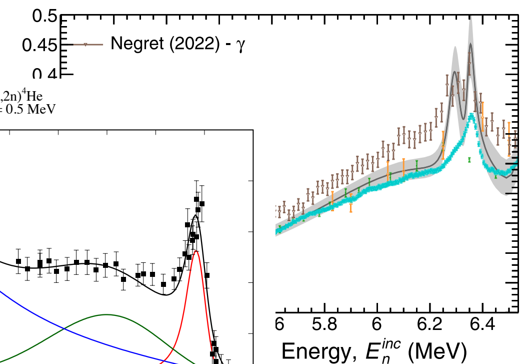

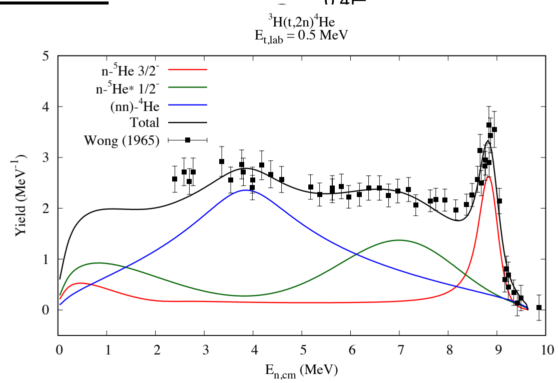

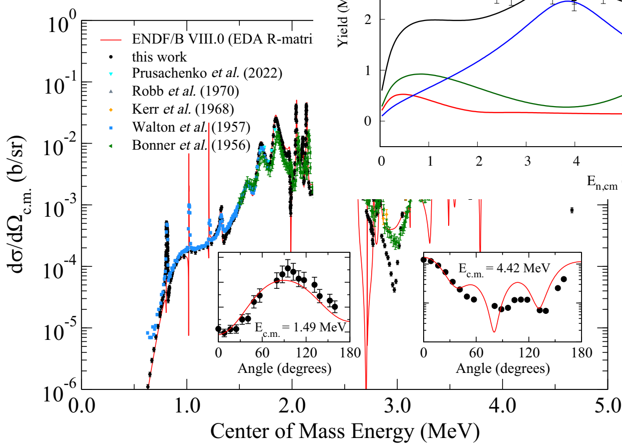

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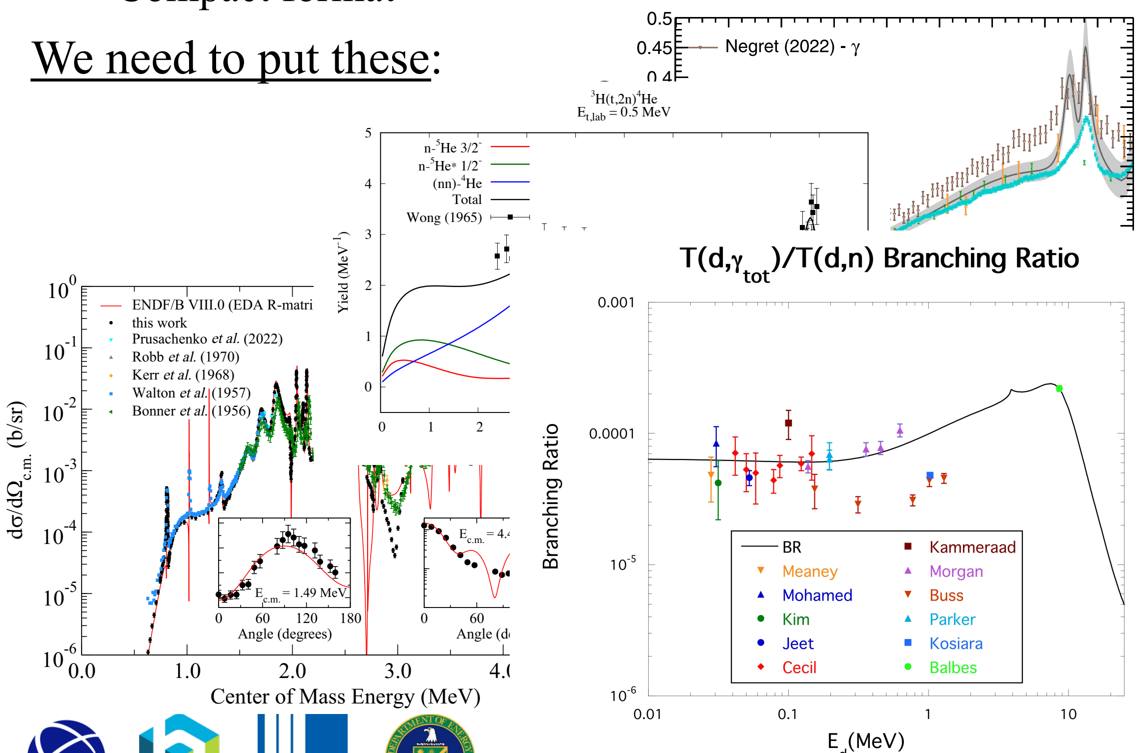

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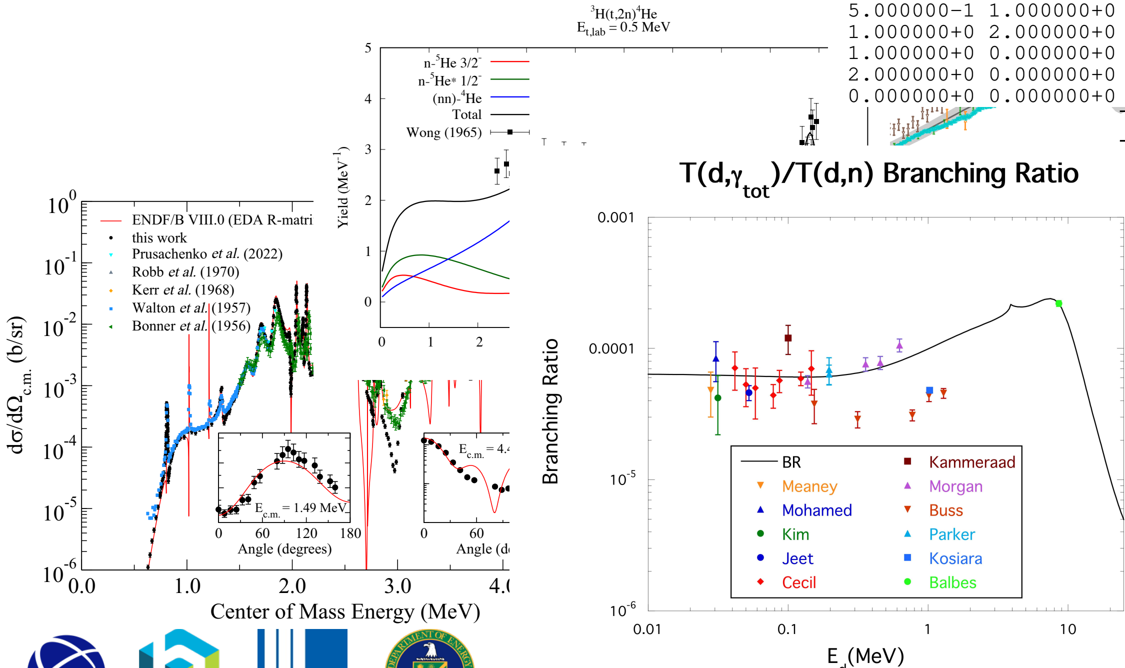


Into something like this (ENDF/B):

```
1.003000+3 3.96713130          0          0          1          0 131 2151
1.003000+3 1.000000+0          0          0          1          0 131 2151
1.000000+0 7.000000+6          1          7          0          1 131 2151
0.000000+0 0.000000+0          1          4          7          0 131 2151
0.000000+0 0.000000+0          2          0         24          4 131 2151
1.99625582 2.98959610          1          1 1.000000+0 5.000000-1 131 2151
0.000000+0          1          1          2          1          1 131 2151
1.000000+0 3.96713130          0          2 5.000000-1 0.000000+0 131 2151
17589245.6          1          1         50          1          1 131 2151
1.500000+0          0          0          0         24          4 131 2151
1.000000+0 0.000000+0 1.500000+0-2.786400-1 5.100000+0 5.100000+0 131 2151
1.000000+0 2.000000+0 1.500000+0 0.000000+0 5.100000+0 5.100000+0 131 2151
1.000000+0 2.000000+0 5.000000-1 0.000000+0 5.100000+0 5.100000+0 131 2151
2.000000+0 2.000000+0 5.000000-1-5.570000-1 3.000000+0 3.000000+0 131 2151
0.000000+0 0.000000+0          0          2         12          2 131 2151
12967.2935 7421.20304 0.000000+0 0.000000+0 215.121811 0.000000+0 131 2151
5996159.03 374.041394 0.000000+0 0.000000+0 1175.09738 0.000000+0 131 2151
5.000000-1 1.000000+0          0          0         18          3 131 2151
1.000000+0 2.000000+0 1.500000+0-1.000000+0 5.100000+0 5.100000+0 131 2151
1.000000+0 0.000000+0 5.000000-1-1.000000+0 5.100000+0 5.100000+0 131 2151
2.000000+0 0.000000+0 5.000000-1-1.000000+0 3.000000+0 3.000000+0 131 2151
0.000000+0 0.000000+0          0          1          6          1 131 2151
```

R-matrix formalism

Q: What does R-matrix evaluation buy for you?

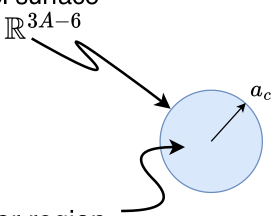
A: Unitarity, Causality, Uncertainty Quantification in a <u>compact</u> format.

<u>Exterior region</u> $r \to \infty$

$$|\Psi_c\rangle = |\mathscr{I}_c\rangle - \sum_{c'} |\mathscr{O}_{c'}\rangle S_{c'c}$$

$$S_{cc'} = \delta_{cc'} + 2i\, T_{cc'}$$

Channel surface $\mathscr{S}_c \in \mathbb{R}^{3A-6}$



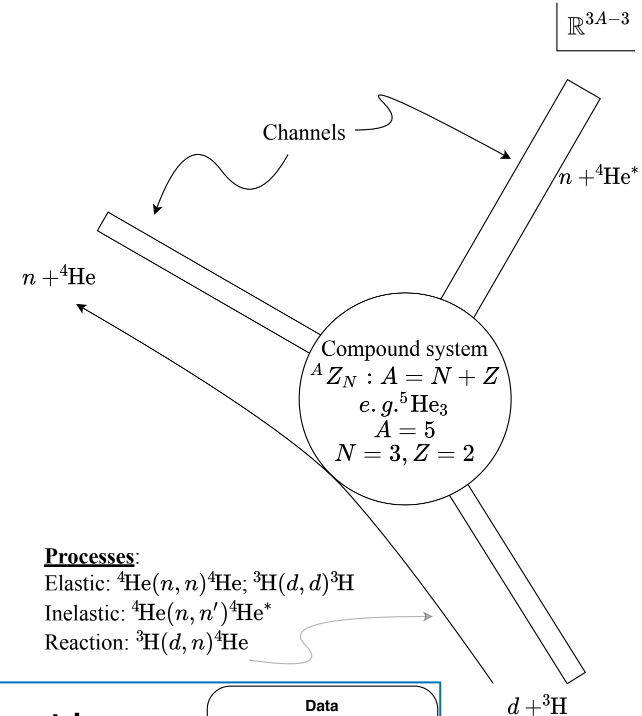
<u>Interior region</u>

$$[H + \mathscr{L}_B]|\lambda\rangle = E_\lambda |\lambda\rangle$$

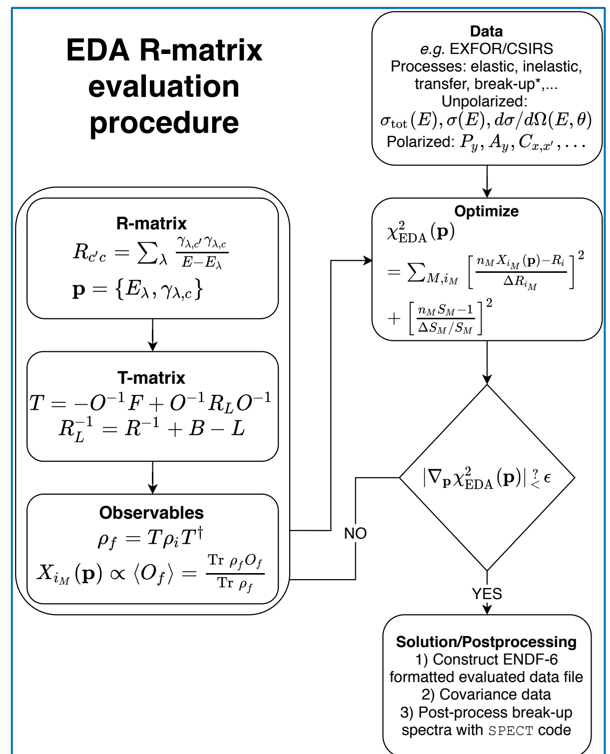
$$|\Psi\rangle = [H + \mathscr{L}_B - E]^{-1} \mathscr{L}_B |\Psi\rangle$$

$$\mathscr{L}_B = \sum_c \frac{i a_c}{2 m_c} |a_c\rangle\langle a_c| (\hat{p}_r + i B_c)$$

$$R_{B,c'c} = \langle c'|[H + \mathscr{L}_B - E]^{-1}|c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$



<u>Processes</u>:
Elastic: ${}^4\mathrm{He}(n,n){}^4\mathrm{He}$; ${}^3\mathrm{H}(d,d){}^3\mathrm{H}$
Inelastic: ${}^4\mathrm{He}(n,n'){}^4\mathrm{He}^*$
Reaction: ${}^3\mathrm{H}(d,n){}^4\mathrm{He}$



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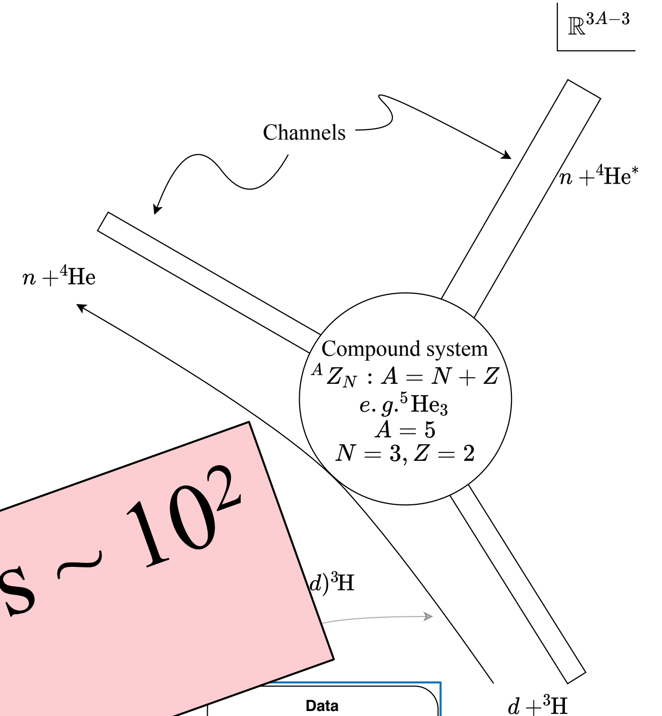
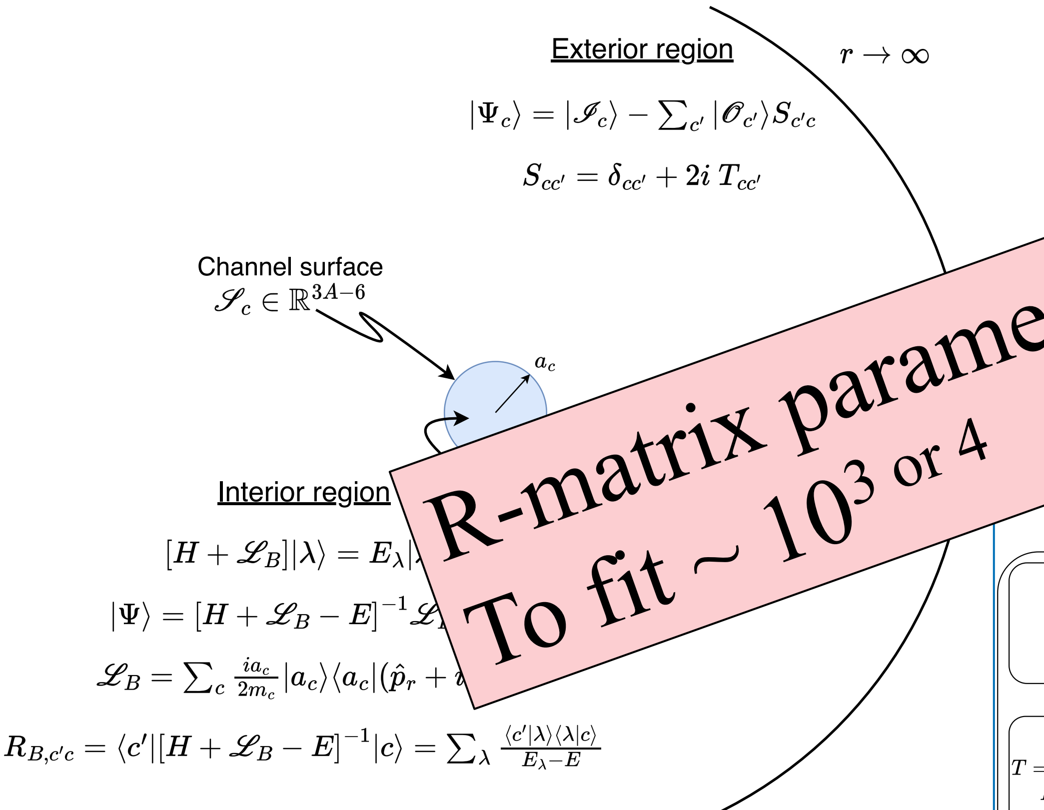
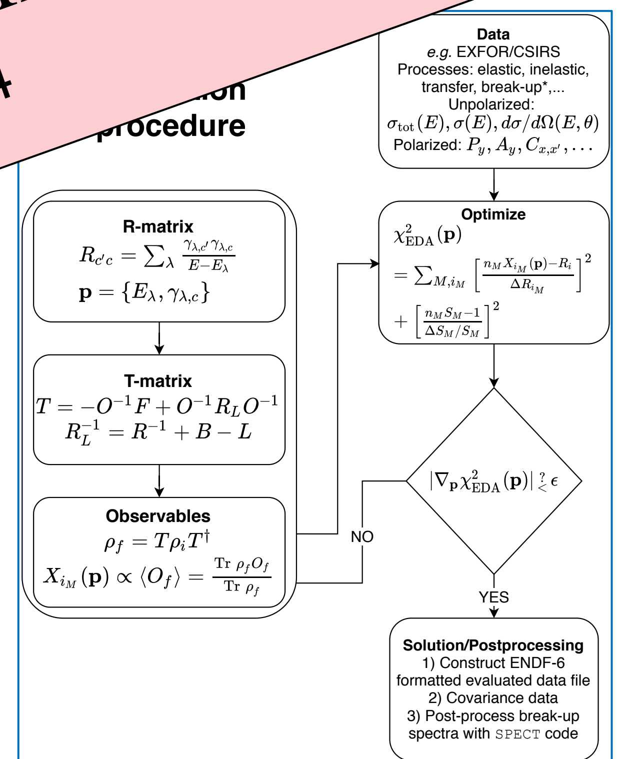




R-matrix parameters ~ 10^2

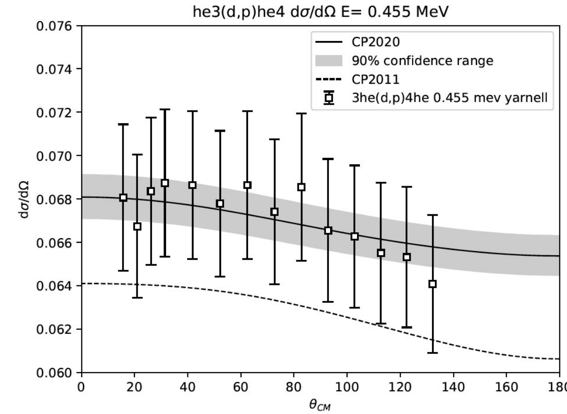
To fit ~ $10^{3 \text{ or } 4}$

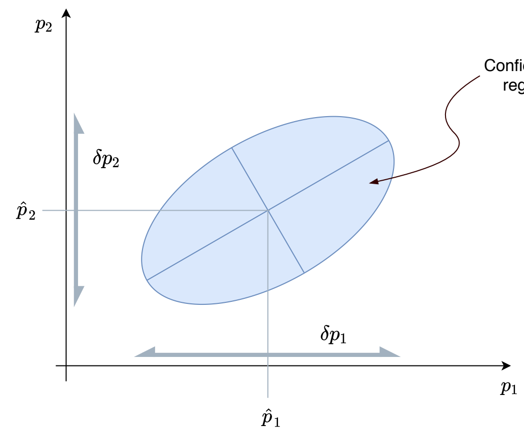


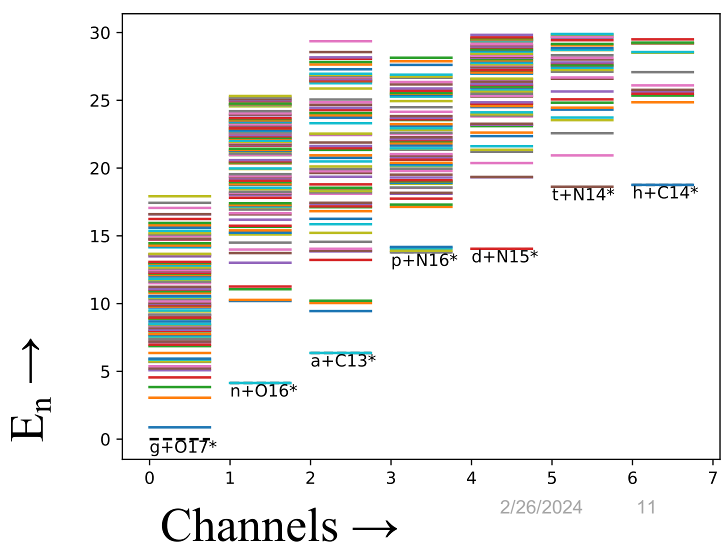
R-matrix formalism

Data generated, constraints & limitations

- A "Solution" generates complete compound system data
  - T matrix ⟹
    - Cross sections
    - Angular distributions
    - Polarization observables
    - All observables $A(z_1,z_2)B$
  - Parameter covariance matrix } uncertainties
  - Sensitivities } uncertainties
- Constraints/limitations
  - Need the observed data
    - Cross section, angular distributions, ***polarization information***
  - With good kinematical coverage; shape-consistent with datasets from other experiments
  - "High" energies ≥ 14.1 MeV neutrons
    - Breakup reactions
      - And these are compound-system dependent
    - Large numbers of channels







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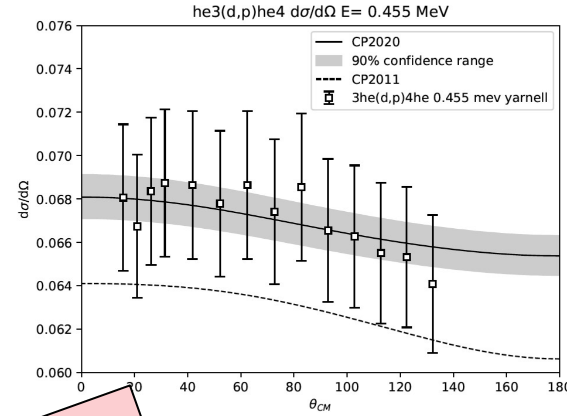
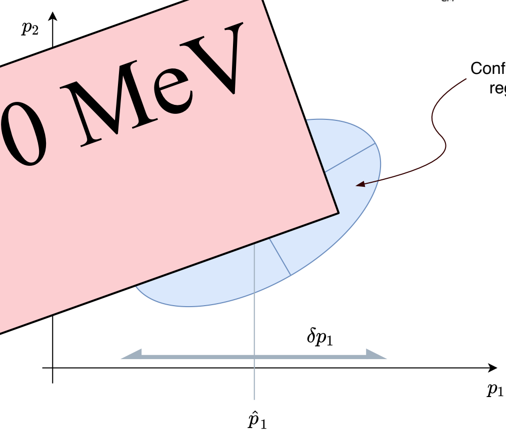
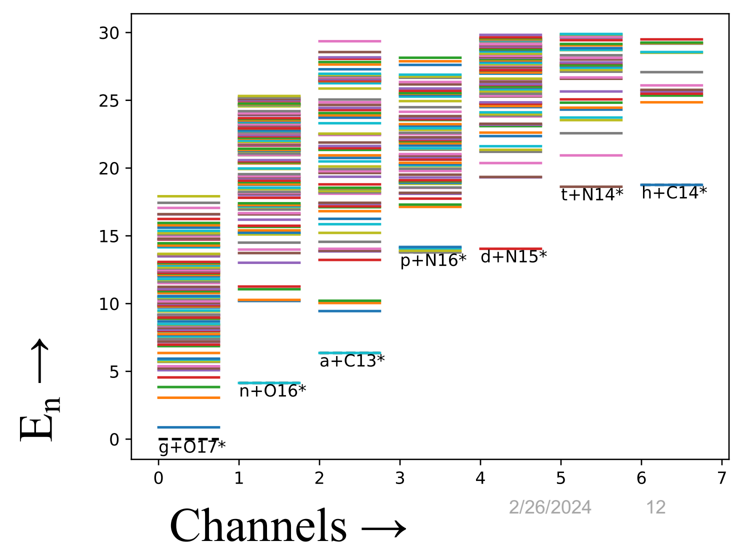
But we need 14.1—30 MeV neutrons!!!



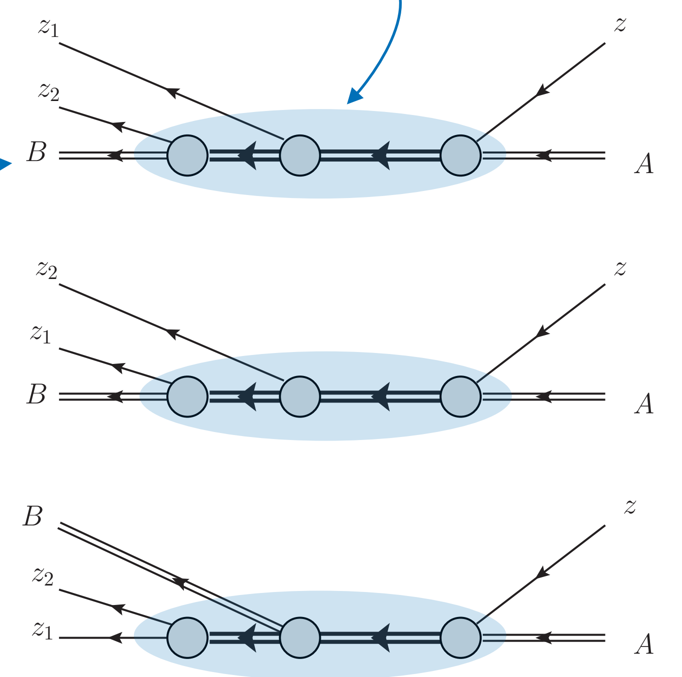




Resonant model for breakup

How we solve the high-energy problem

Objective:
- predictive model for breakup
- use existing R-matrix parameters



$$\text{Breakup Reactions}$$

$$\begin{aligned} &A(z, z_1 z_2)B \\ =&A(z,(z_2B))z_1 \\ +&A(z,(z_1B))z_2 \\ +&A(z,(z_1z_2))B \end{aligned}$$

$$|\psi^+_{\mathbf{k}_0}\rangle = |\chi_{\mathbf{k}_0}\rangle + \mathscr{G}^+_i H'_i |\psi^+_{\mathbf{k}_0}\rangle$$

$$\mathscr{G}^+_i(E) = \frac{1}{2\pi i}\int_C dz\, G^{(x)+}_i(z) G^{(r)+}_{0,i}(E-z),$$

$$|\psi^+_{\mathbf{k}_0}\rangle \doteq -\left(\frac{2\pi\bar{\mu}_i}{\hbar^2}\right)^{1/2}\int_0^\infty dE_{\mathbf{q}_i}\,\frac{e^{ik_ir_i}}{r_i\sqrt{k_i}}|\phi^-_{\mathbf{q}_i}\rangle\langle\phi^-_{\mathbf{q}_i}|H'_i|\psi_{\mathbf{k}_0}\rangle,$$

$$= \int_0^\infty dE_{\mathbf{q}_i}\sqrt{\frac{2\bar{\mu}_i}{\pi\hbar^2 k_i}}\,\frac{e^{ik_ir_i}}{r_i}|\phi^-_{\mathbf{q}_i}\rangle \tilde{T}^{(2)}_{\mathbf{q}_i\mathbf{k}_i,\mathbf{k}_0},$$

Resonant model for breakup

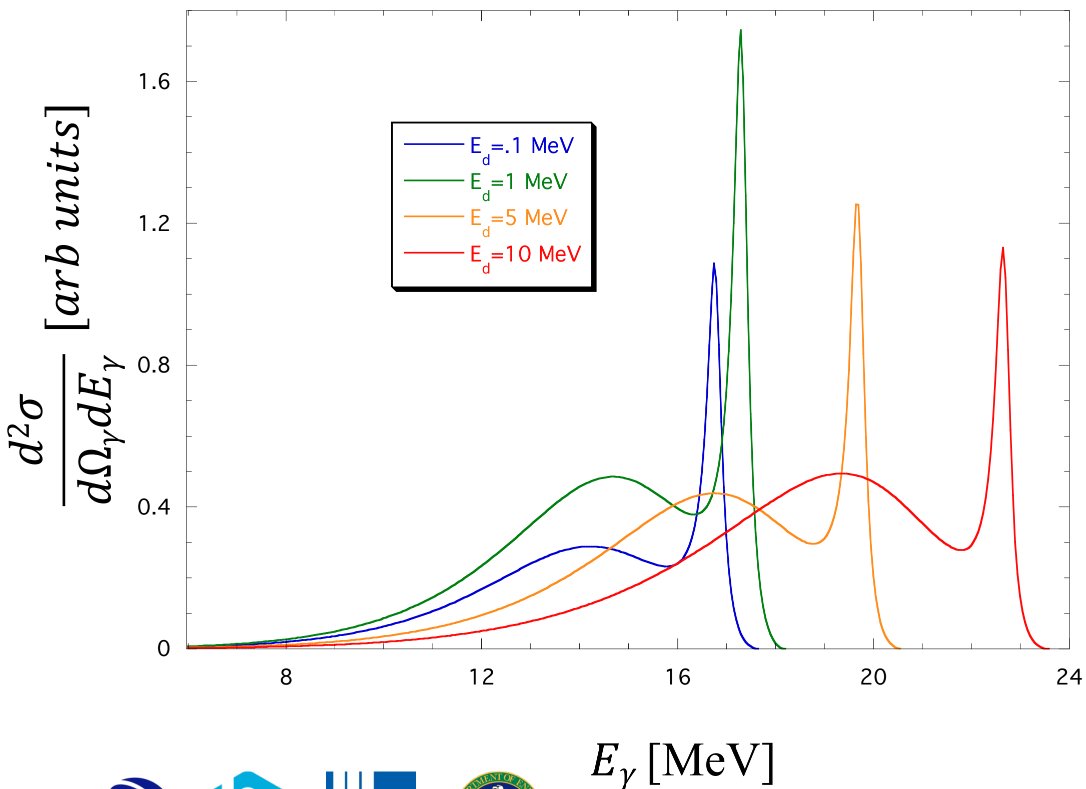
How we solve the high-energy problem

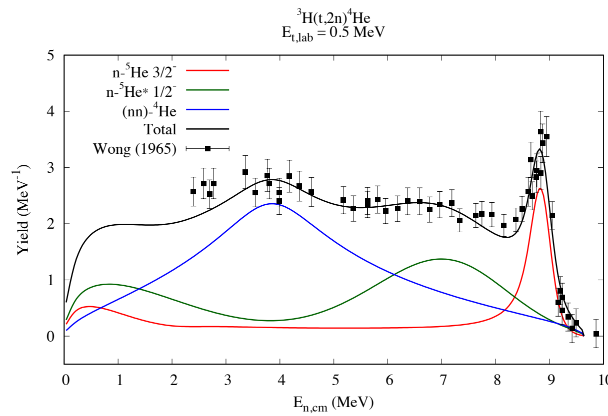
- Applications
  - $^{3}H(d,n\gamma)^{4}He$
  - $^{3}H(t,2n)^{4}He$

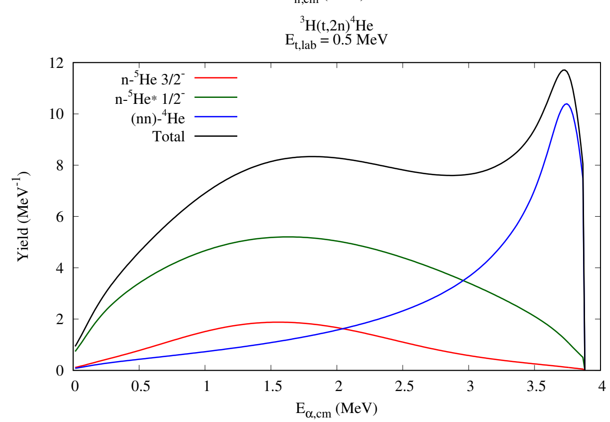
SPECT code calculation

- Employs Faddeev-like resonance model
- Relativistic kinematics necessary for γ production

$^{3}H(d,n\gamma)^{4}He$ spectrum @ 90°







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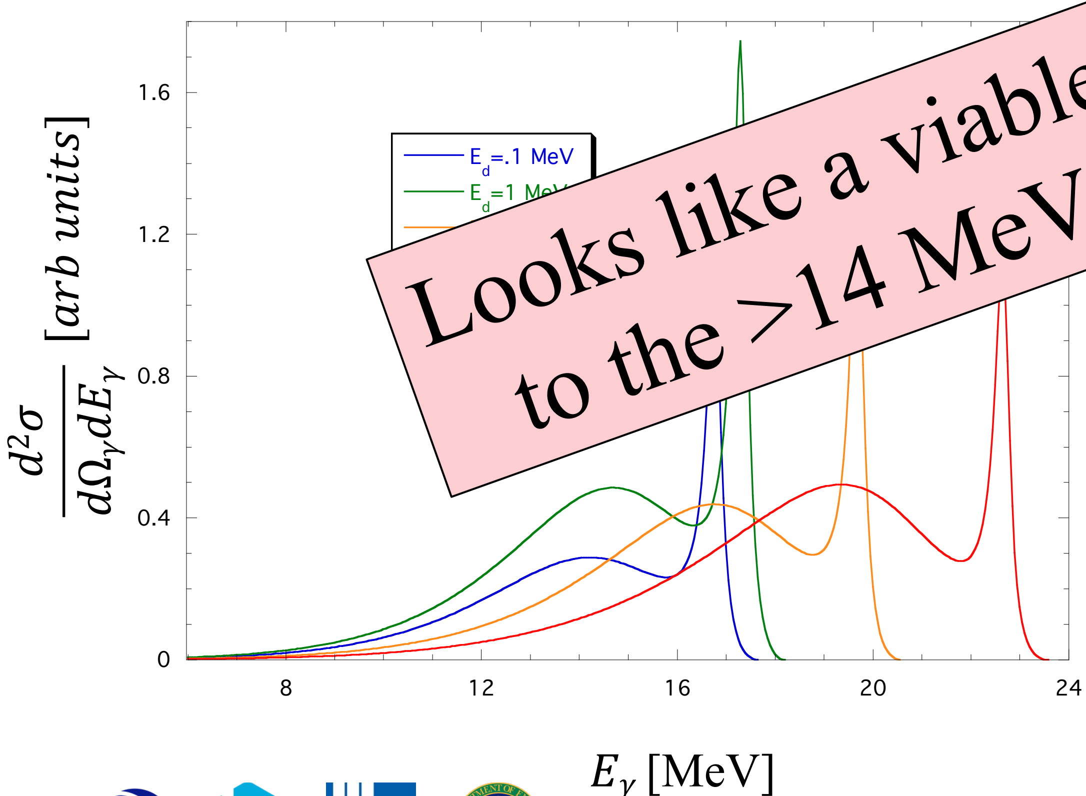
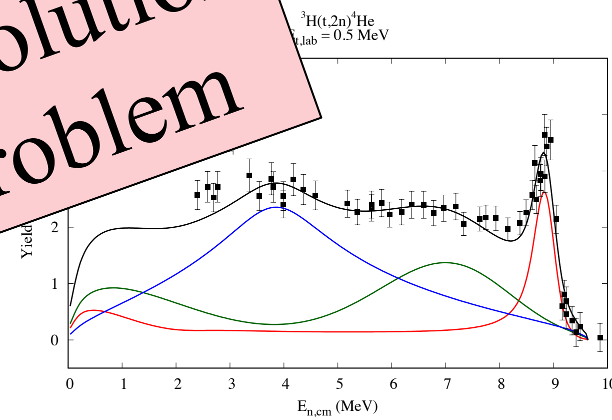
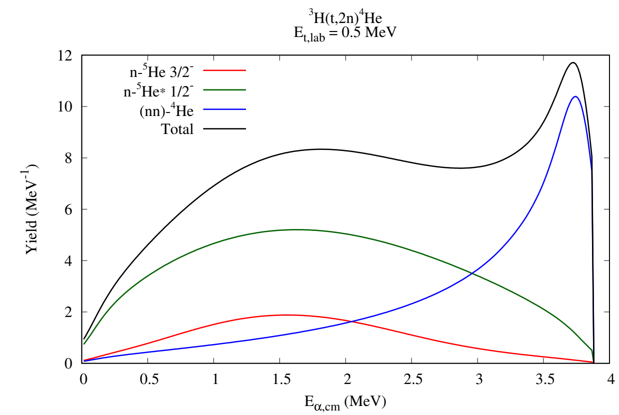


Looks like a viable solution to the >14 MeV problem





LANL light-element program

- All compound systems A<20 (and a few above)
- Recent work:

Projectile\Target	^{1}H	^{2}H	^{3}H	^{3}He	^{4}He	^{6}Li	^{7}Li
n	2020	VIII.0	VIII.0	VIII.0	VIII.0	2020	VIII.0
p	2020	VIII.0	VIII.0	VIII.0	2020	VIII.0	VIII.0
d		VIII.0	VIII.0	2020	VIII.0^{a}	VIII.0	VIII.0
t			VIII.0	VIII.0	2020	VIII.0	TENDL09
h(^{3}He)				VIII.0	VIII.0	VIII.0	TENDL09
α					VIII.0	TENDL09	TENDL09

^{11}B (α+^{7}Li, α+^{7}Li*, t+^{8}Be, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)
^{13}C (n+^{12}C, n+^{12}C*)
^{14}C (n+^{13}C)
^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)
^{16}O (g+^{16}O, α+^{12}C)
^{17}O (n+^{16}O, α+^{13}C)
^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)

- ~30 Compound systems
  - not all shown
- ~100 Reactions

R-matrix evaluation status

Materials of interest for fusion neutronics

- Lowest n breakup thresholds
  - Target material
  - Products
  - Neutron threshold energy
  - Maximum energy in our current EDA evaluations
- Negative threshold denotes exothermic ($Q > 0$) reaction
- Maximum evaluation energy is usually lower than the breakup threshold
  - If not, we've started to push into the breakup region

Material	Products	$E_{n,\mathrm{thr}}$ (MeV)	$E^{\mathrm{EDA}}_{n,\max}$ (MeV)
$n+^{2}\mathrm{H}$	$2np$	3.34	3.0
$n+^{3}\mathrm{H}$	$2nd$	8.35	10.5
$n+^{6}\mathrm{Li}$	$nd\alpha$	1.72	7.0
$n+^{7}\mathrm{Li}$	$nt\alpha$	2.82	NA
$n+^{7}\mathrm{Be}$	$pt\alpha$	0.94	1.4
$n+^{9}\mathrm{Be}$	$2n2\alpha$	1.75	5.0
$n+^{10}\mathrm{B}$	$t2\alpha$	−0.32	1.1
$n+^{11}\mathrm{B}$	$n\alpha^{7}\mathrm{Li}$	9.46	NA
$n+^{12}\mathrm{C}$	$n3\alpha$	7.89	10.0
$n+^{13}\mathrm{C}$	$2n^{12}\mathrm{C}$	5.33	11.0
$n+^{13}\mathrm{N}$	$np^{12}\mathrm{C}$	2.09	NA
$n+^{14}\mathrm{N}$	$np^{13}\mathrm{C}$	8.09	2.5
$n+^{16}\mathrm{O}$	$n\alpha^{12}\mathrm{C}$	7.61	8.0

- Much of our current effort is focused on pushing the maximum energy of the evaluation $E^{EDA}_{n,max}$ to energies higher than those show here with > 14.1 MeV being the target.

SBEND Collaboration (BNL/LANL/LLNL)

Priority evalations

- Materials of interest
  - **First priority**
    - H, C, N, O
  - **Follow-up**
    - He, Li, Be, B

Category	Material	SBEND Elements
Structural	Al, steel, AM material	H, C, N, O
Controlled substances	Conventional explosives, pharmaceuticals, chemical agents, SNM	H, C, N, O, F, P
Intervening (shielding)	Poly, H_2O, *n* abs, Pb, W	H, Li, Be, B, C, O
Detector	Org & inorg scint, semicon, housings, PMT	He, He, C, O
Source	Detector housing, source reactions	Li, Be

- Elemental processes of interest
  - SBEND initial prioritization
    - subject to need
  - DOE/SC & NNSA motivation

Priority evaluations	DOE-SC user interest	NNSA user interest
$^{1}H(n,n)^{1}H$; $^{1}H(n,\gamma)^{2}H$; $^{2}H(\gamma,n)^{1}H$	Reference/monitor cross section; BBN	Reference/monitor for various actinides, *e.g.* $^{235}U(n,f)$; Non-proliferation/interrogation
$^{6}Li(d,\alpha)^{4}He$; $^{7}Li(p,\gamma/\gamma^{*})^{8}Be$	BSM physics; BBN	Nuclear security
$^{12}C(n,n'\gamma)^{12}C$; $^{12}C(\alpha,\gamma)^{16}O$; $^{12}C(\alpha,\alpha'\gamma)^{12}C$	Stellar nucleosynthesis; nuclear structure	Secondary γ-rays non-proliferation/interrogation
$^{13}C(\alpha,\gamma)^{17}O$; $^{13}C(\alpha,\gamma)^{16}O$; $^{13}C(\alpha,\alpha'\gamma)^{13}C$	Stellar nucleosynthesis; nuclear structure; Neutrino-detection backgrounds	Secondary γ-rays non-proliferation/interrogation
$^{14}N(n,n)^{14}N$; $^{14}N(n,p)^{14}C$; $^{14}N(n,\alpha)^{11}B$; $^{14}N(n,n'\gamma)^{14}N$	Stellar nucleosynthesis; nuclear structure	Secondary γ-rays non-proliferation/interrogation
$^{15}N(n,n'\gamma)^{15}N$; $^{15}N(p,\alpha'\gamma)^{12}C$;	Stellar nucleosynthesis; nuclear structure	Secondary γ-rays non-proliferation/interrogation
$^{16}O(n,\alpha)^{13}C$; $^{16}O(\gamma^{*},\alpha)^{12}C$; $^{16}O(n,n')^{16}O^{*}$; $^{16}O(n,n'\gamma)^{16}O$;	Stellar nucleosynthesis; nuclear structure; Neutrino-detection backgrounds	Secondary γ-rays non-proliferation/interrogation

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    - H, C, N, O
  - **Follow-up**
    - He, Li, Be, B

Category	Material	SBEND Elements
Structural	Al, steel, AM material	H, C, N, O
Controlled substances	Conventional explosives, pharmaceuticals, chemical agents, SNM	H, C, N, O, F, P
Intervening (shielding)	Poly, H_2O, *n* abs, Pb, W	H, Li, Be, B, C, O
Detector	Org & inorg scint … PMT	He, He, C, O
Source	[illegible]	Li, Be

- Elemental processes of interest
  - SBEND ini… prioritizatio…
    - subject to ne…
  - DOE/SC & NNSA motivation

Priority ev…	…erest	NNSA user interest
^{1}H…	…ce/monitor cross section; BBN	Reference/monitor for various actinides, *e.g.* $^{235}U(n,f)$; Non-proliferation/interrogation
…$(p,\gamma/\gamma^*)^{8}Be$	BSM physics; BBN	Nuclear security
…$\gamma)^{12}C$; $^{12}C(\alpha,\gamma)^{16}O$; …$C(\alpha,\alpha'\gamma)^{12}C$	Stellar nucleosynthesis; nuclear structure	Secondary γ-rays non-proliferation/interrogation
$^{13}C(\alpha,\gamma)^{17}O$; $^{13}C(\alpha,\gamma)^{16}O$; $^{13}C(\alpha,\alpha'\gamma)^{13}C$	Stellar nucleosynthesis; nuclear structure; Neutrino-detection backgrounds	Secondary γ-rays non-proliferation/interrogation
$^{14}N(n,n)^{14}N$; $^{14}N(n,p)^{14}C$; $^{14}N(n,\alpha)^{11}B$; $^{14}N(n,n'\gamma)^{14}N$	Stellar nucleosynthesis; nuclear structure	Secondary γ-rays non-proliferation/interrogation
$^{15}N(n,n'\gamma)^{15}N$; $^{15}N(p,\alpha'\gamma)^{12}C$;	Stellar nucleosynthesis; nuclear structure	Secondary γ-rays non-proliferation/interrogation
$^{16}O(n,\alpha)^{13}C$; $^{16}O(\gamma^*,\alpha)^{12}C$; $^{16}O(n,n')^{16}O^*$; $^{16}O(n,n'\gamma)^{16}O$;	Stellar nucleosynthesis; nuclear structure; Neutrino-detection backgrounds	Secondary γ-rays non-proliferation/interrogation

Tell us your priorities!

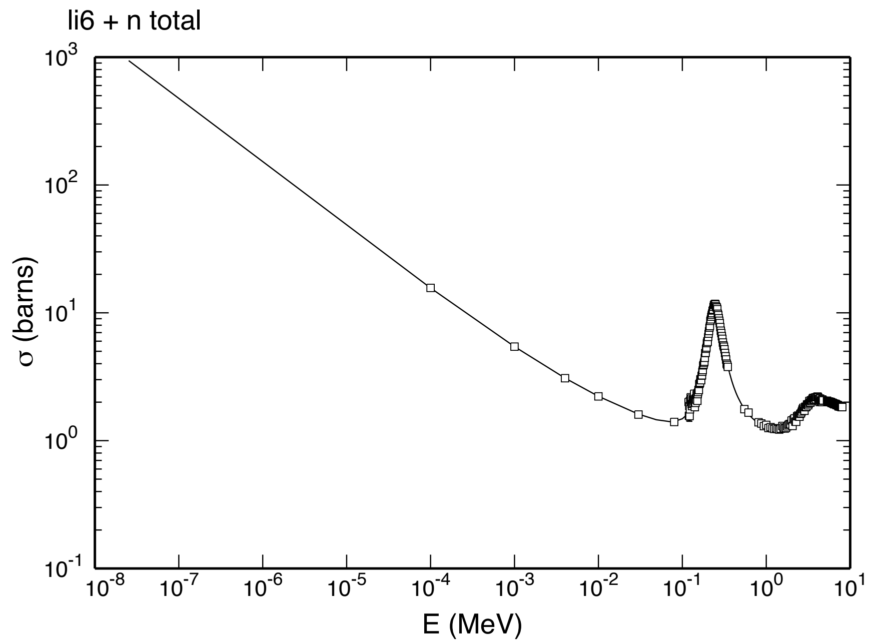
Thanks in advance for your questions & support

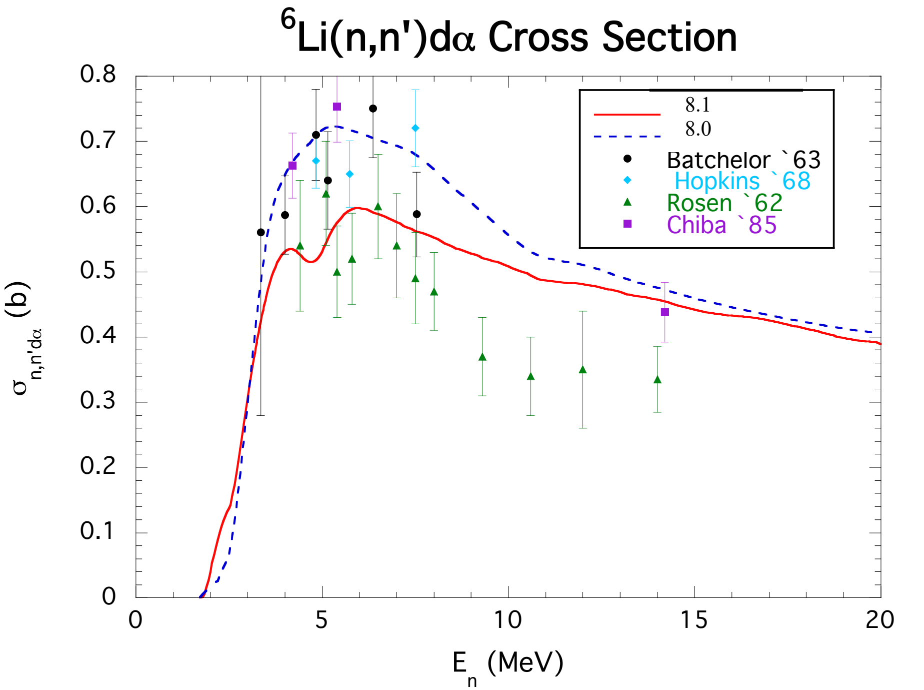
n+^{6}Li

R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VIII.0
  - upper energy limit $E_n \leq 4.3$ MeV
  - configuration: t+^{4}He, n+^{6}Li, n+^{6}Li*(3^{+}; 2.19 MeV), d+^{5}He*($3/2^{-}$)
  - ~3,800 data points; $\chi^2/dof \approx 1.36$
  - formatting changes: MF=4→MF=6; MT=24→41 (n,2np)

- Updated evaluation (accepted for ENDF/B-VIII.1)
  - upper energy limit $E_n \leq 8.0$ MeV
  - new configuration = old config + inelastic: n_2+^{6}Li(0^{+}; 3.56 MeV)
  - new data covering all channels
  - corrected ^{6}Li(n,n'd)^{4}He spectra





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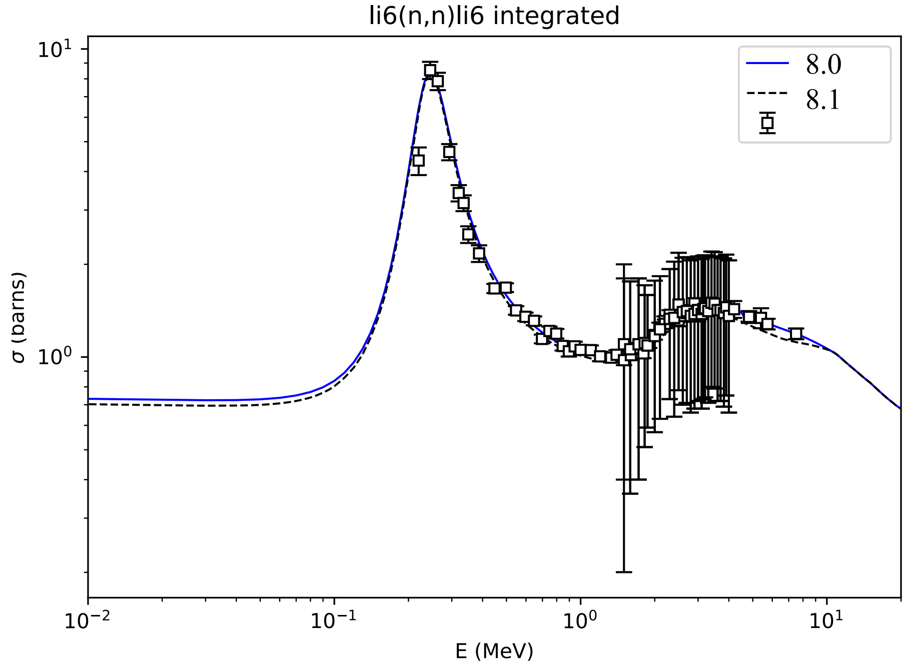

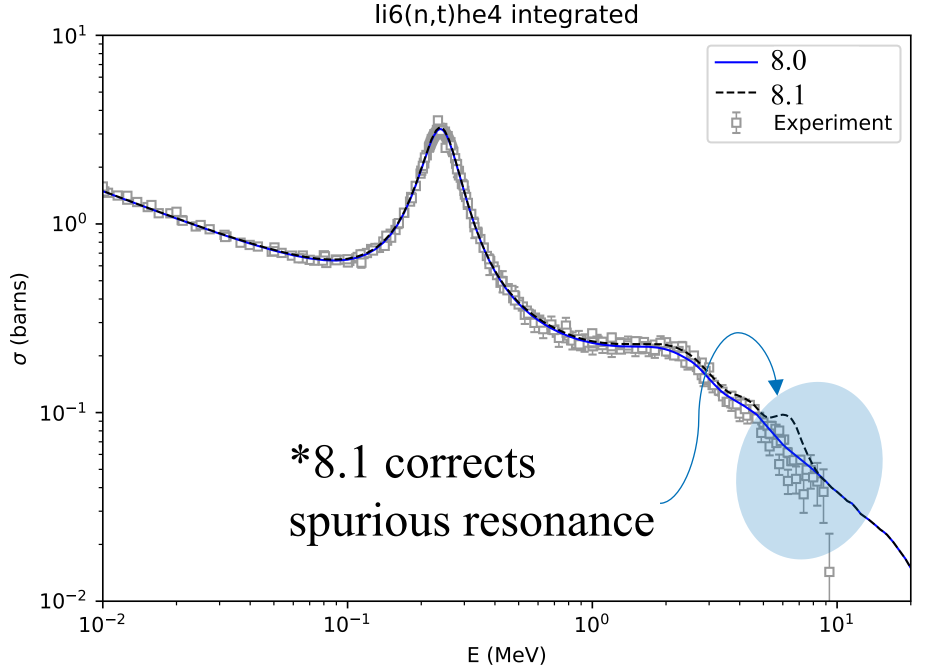

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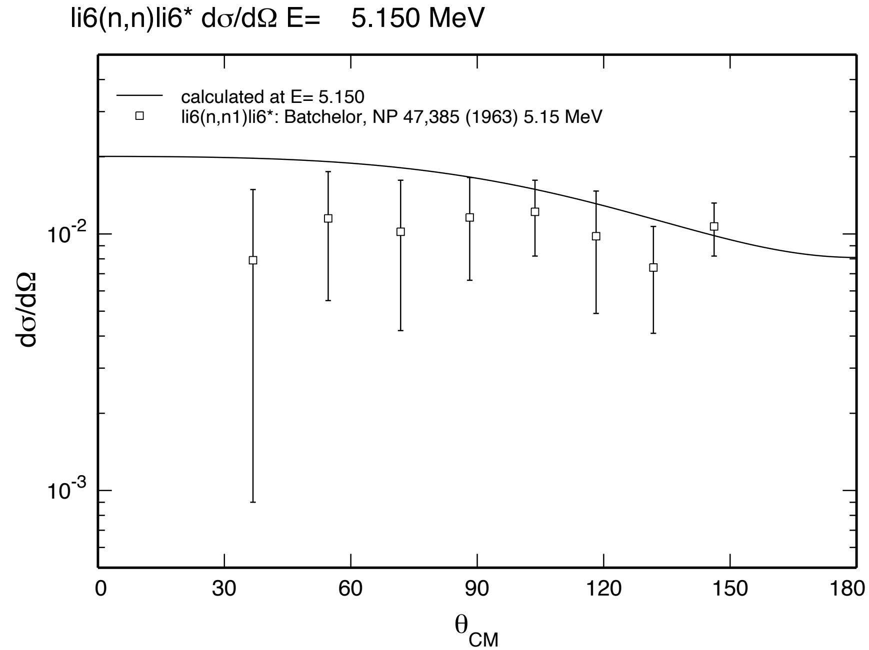
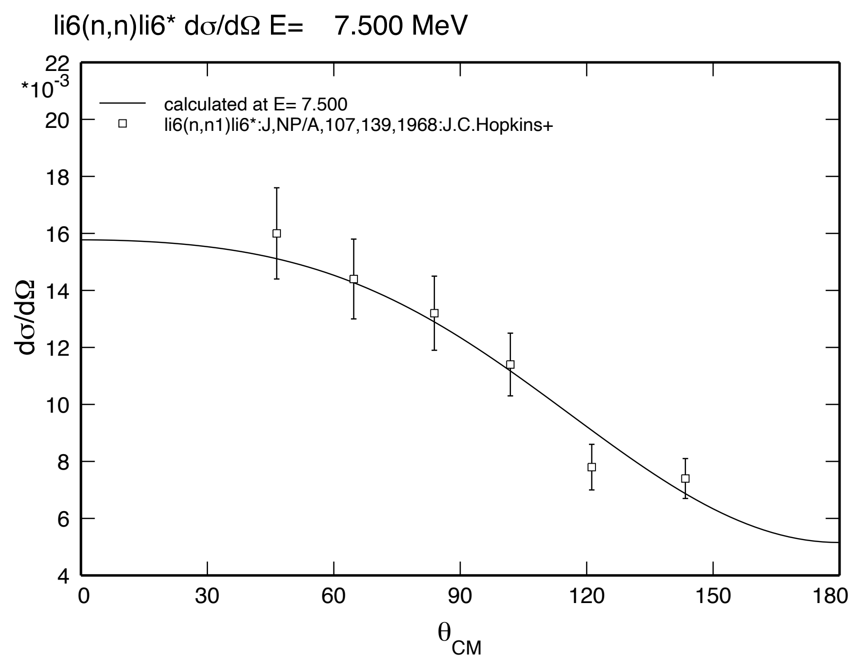




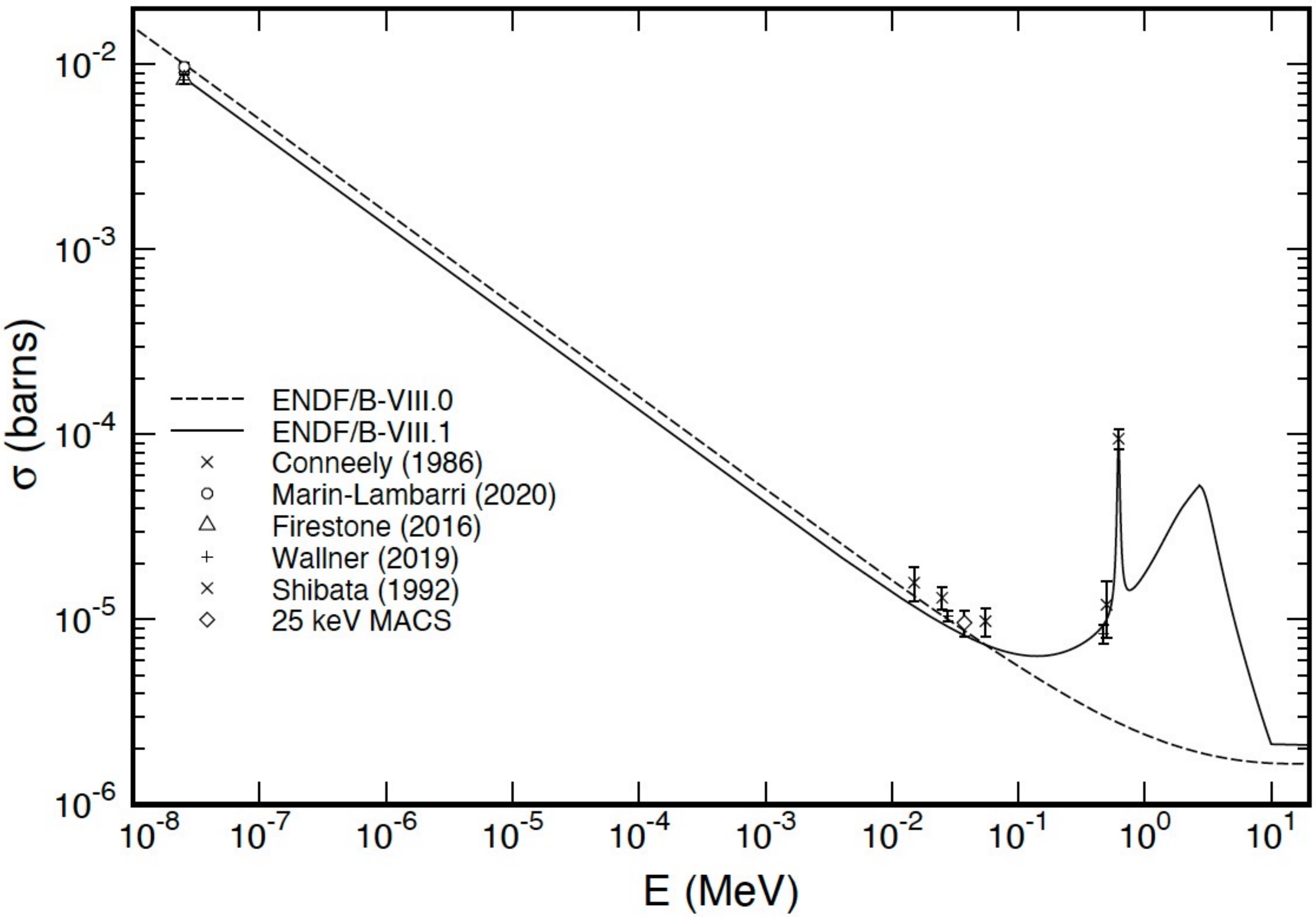
n+^{9}Be

R-matrix evaluation update/extension

- New evaluation highlights
  - Added ^{9}Be(n,γ)^{10}Be evaluation
  - (new evaluation work on (n,el), (n,inl), (n,α) will hold for ENDF/B-IX.0 when (n,2nα) is re-evaluated)

Improved perf. on FLATTOP

ENDF/B	VIII.0	VIII.1
C/E	0.134	0.919



E		$\sigma_{(n,\gamma)}$		$\delta\sigma_{(n,\gamma)}$		Ref.
0.0253	eV	8.49	mb	0.34	mb	[75]
0.0253	eV	9.70	mb	0.53	mb	[79]
0.0253	eV	8.27	mb	0.13	mb	[77]
0.0253	eV	8.31	mb	0.52	mb	[78]
15.0	keV	15.81	μb	3.3	μb	[76]
30.0	keV	13.00	μb	1.8	μb	[76]
55.0	keV	9.79	μb	1.7	μb	[76]
27.8	keV	10.44	μb	0.63	μb	[78]
473	keV	8.4	μb	1.0	μb	[78]
500	keV	12.02	μb	4.1	μb	[76]
622	keV	94.80	μb	12.1	μb	[76]

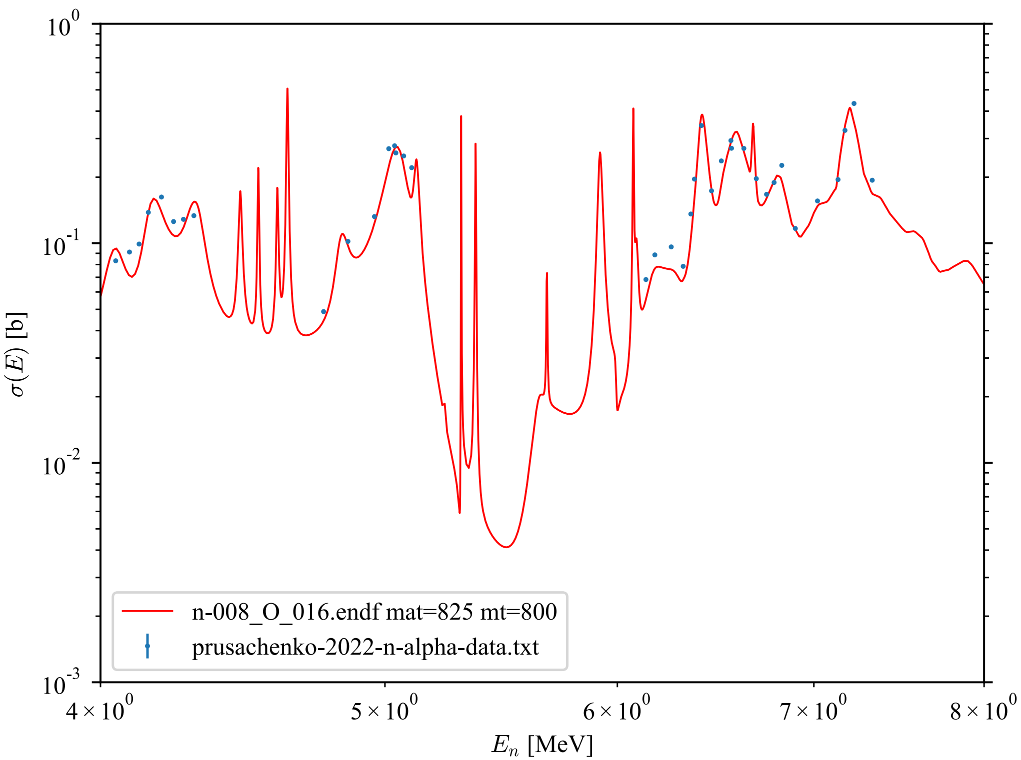
- [75] Conneely (1986)
- [76] Shibata (1992)
- [77] Firestone (2016)
- [78] Wallner (2019)
- [79] Marin-Lambarri (2020)

n+^{16}O

Evaluation adjustment for $^{16}O(n,\alpha_i)^{13}C^*$

- Abbreviated history
  - concern that $^{16}O(n,\alpha)^{13}C$ absorption in ENDF/B-VIII.0 too large
  - LANL/EDA R-matrix fit considers $E_n \lesssim 7.0$ MeV
  - Excited states $E_n > 5.6$ MeV
- New data
  - supports ENDF/B-VIII.0 to 7.0 MeV
    - **Prusachenko et al. IPPE 2022**
    - H.-Y. Lee, S. Kuvin, et al. 2023
- Implement reduction in (n,α_i)
  - $i = 1,2,3 \leftrightarrow MT = 801,802,803$
  - reduced by factor of 2 to agree with Davis

$^{A}Z_i$ J^π	$E_x(^{13}\text{C})$ (MeV)	$Q_{n\alpha_i}$ (MeV)	E_n (MeV)
$^{13}\text{C}_0$ $\frac{1}{2}^-$	0.0	−2.215	2.355
$^{13}\text{C}_1$ $\frac{1}{2}^+$	3.08944	−5.304	5.639
$^{13}\text{C}_2$ $\frac{3}{2}^-$	3.68451	−5.899	6.271
$^{13}\text{C}_3$ $\frac{5}{2}^+$	3.85381	−6.068	6.451
$^{13}\text{C}_4$ $\frac{5}{2}^+$	6.864	−9.079	9.651



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