



Recent updates to the ${}^6\text{Li}$, ${}^9\text{Be}$ and ${}^{16}\text{O}$ evaluations for ENDF/B-VIII.1

Nuclear Criticality Safety Program—Technical Program Review

M. Paris, G. Hale & Mike Herman (LANL/T-2)

N. Gibson, N. Kleedtke & D. Neudecker (LANL/XCP-5)

Presenter: Bob Little (LANL)

2024 Feb 20—22

LA-UR-24-21184

Outline

- By “recent,” we mean $\gtrsim 2020$
- Overview of R-matrix evaluation procedure
- Evaluation work [for testing see recent NCSP & CSEWG talks]
 - $n+{}^6\text{Li}$
 - $n+{}^9\text{Be}$
 - $n+{}^{16}\text{O}$
- Conclusion

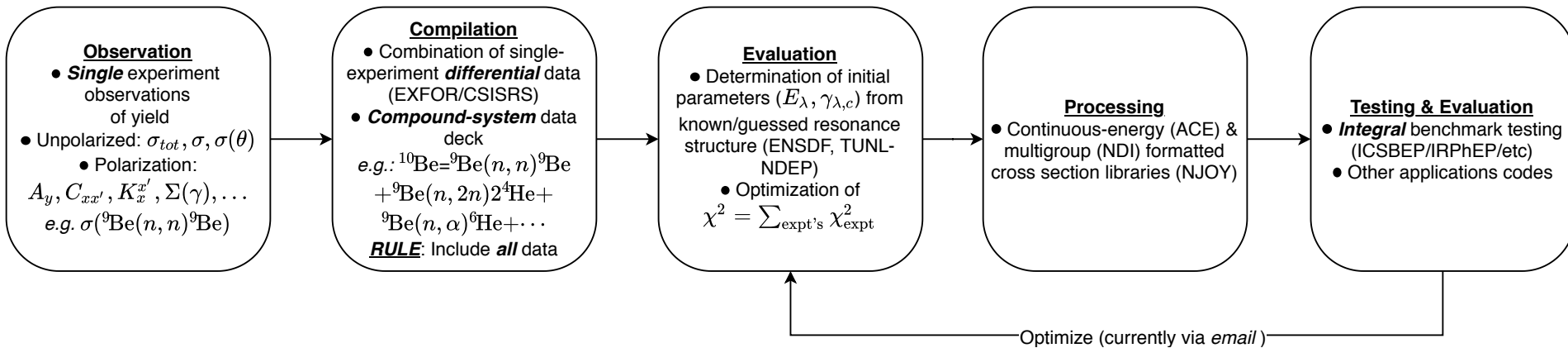


Evaluation pipeline

EDA R-matrix procedure

Nuclear Data Pipeline

EDA cross section evaluation



1. **EDAf90** code handles all types of data [*EXFOR/CSISRS; publications; priv. comm.*]
– total, integrated, diff'l, polarized, unpolarized; neutron- and CP-induced: (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



n+⁶Li

R-matrix evaluation update/extension

- New evaluation highlights

- Upper energy of R-matrix evaluation increased to $E_n \leq 8.0$ MeV
- Additional, inelastic channel ⁶Li(0+; 3.56 MeV)
- Includes new data in all channels
- Spectra ⁶Li(n,n'd)⁴He: corrected formatting error (LCT=1 → LCT=2)

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	1	(n,total)	(0.00, 20.00)
	2	(z,z0)	(0.00, 20.00)
	4	(z,n)	(1.75, 20.00)
	24	(z,2n α)	(4.32, 20.00)
	51	(z,n ₁)	(1.75, 20.00)
	52	(z,n ₂)	(2.34, 20.00)
	...	(z,n _i)	...
	81	(z,n _n)	(18.10, 20.00)
	102	(z, γ)	(0.00, 20.00)
	103	(z,p)	(3.18, 20.00)
	105	(z,t)	(0.00, 20.00)
4		Angular distributions for emitted particles	
	2	(z,z0)	
	24	(z,2n α)	
	51	(z,n ₁)	
	52	(z,n ₂)	
	...	(z,n _i)	
	81	(z,n _n)	
5		Energy distributions for emitted particles	
	24	(z,2n α)	
6		Energy-angle distributions for emitted particles	
	105	(z,t)	

MF	MT	Description	Energy range [MeV]
3		Reaction cross sections	
	1	(n,total)	(0.00, 20.00)
	2	(z,z0)	(0.00, 20.00)
	4	(z,n)	(4.16, 20.00)
	32	(z,nd)	(1.72, 20.00)
	41	(z,2np)	(4.32, 20.00)
	52	(z,n ₂)	(4.16, 20.00)
	102	(z, γ)	(0.00, 20.00)
	103	(z,p)	(3.18, 20.00)
	105	(z,t)	(0.00, 20.00)
4		Angular distributions for emitted particles	
	2	(z,z0)	
6		Energy-angle distributions for emitted particles	
	32	(z,nd)	
	41	(z,2np)	
	52	(z,n ₂)	
	103	(z,p)	
	105	(z,t)	

NB: No change in standards region for ⁶Li(n,t)⁴He



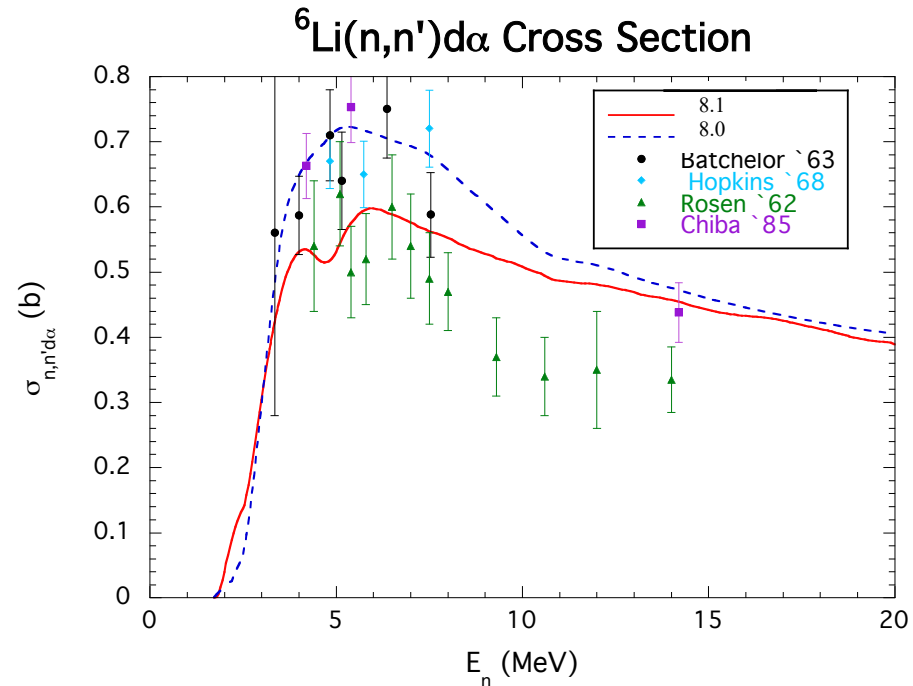
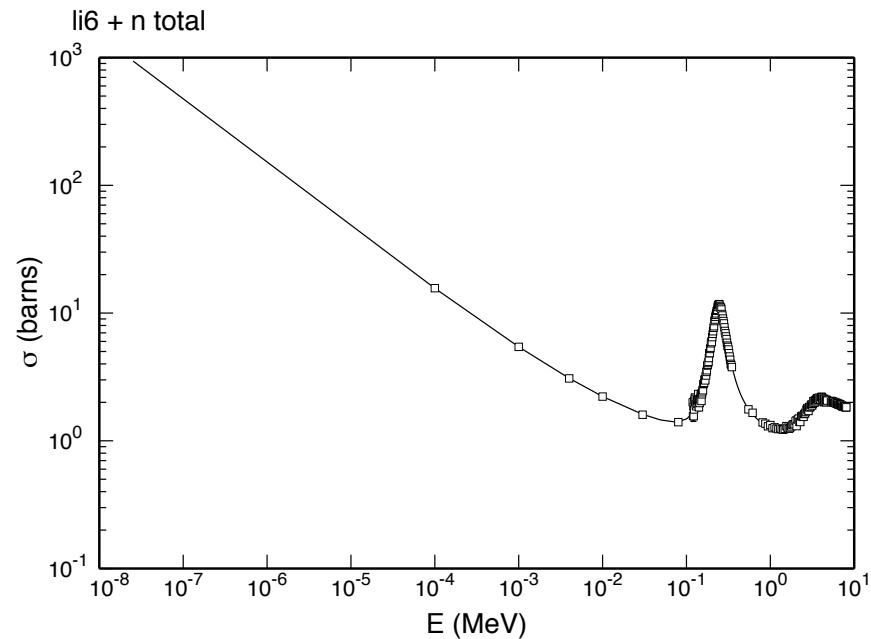
$n+{}^6\text{Li}$

R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VII.1
 - upper energy limit $E_n \leq 4.3$ MeV
 - configuration: $t+{}^4\text{He}$, $n+{}^6\text{Li}$, $n+{}^6\text{Li}^*(3^+; 2.19 \text{ MeV})$, $d+{}^5\text{He}^*(3/2^-)$
 - $\sim 3,800$ data points; $\chi^2/dof \approx 1.36$
 - formatting changes: MF=4 \rightarrow MF=6; MT=24 \rightarrow 41 (n,2np)

- Updated evaluation (submitted for ENDF/B-VIII.1 β 1)

- upper energy limit $E_n \leq 8.0$ MeV
- new configuration = old config + inelastic: $n_2+{}^6\text{Li}(0^+; 3.56 \text{ MeV})$
- new data covering all channels
- corrected ${}^6\text{Li}(n,n'd){}^4\text{He}$ spectra



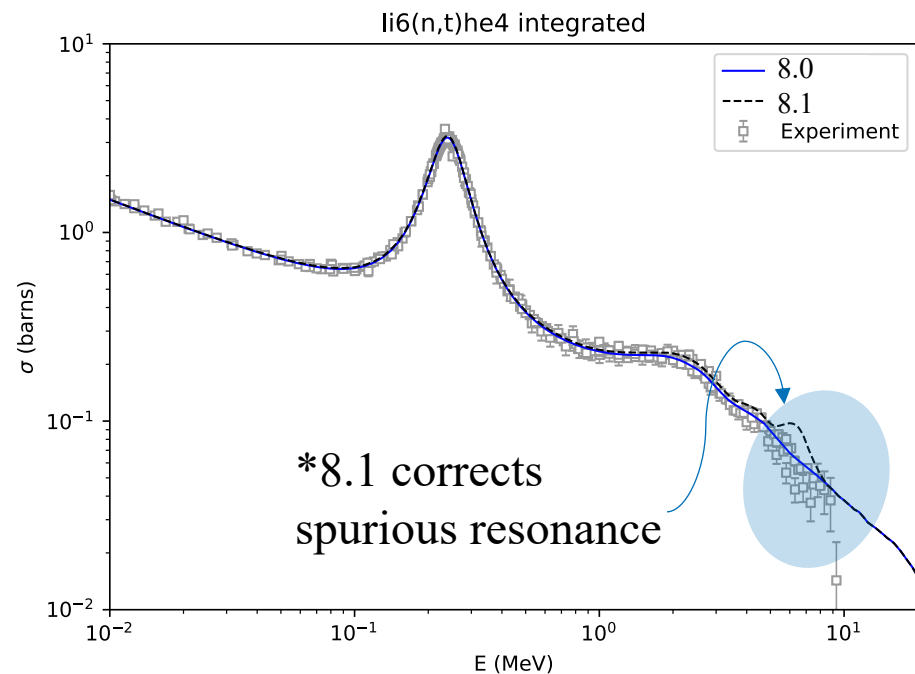
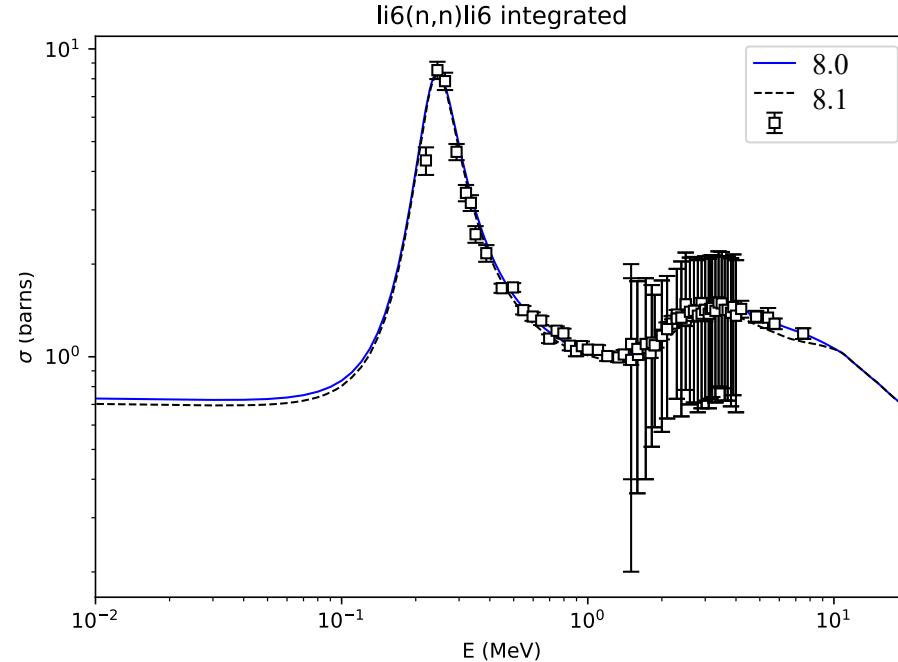
$n+{}^6\text{Li}$

R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VII.1
 - upper energy limit $E_n \leq 4.3$ MeV
 - configuration: $t+{}^4\text{He}$, $n+{}^6\text{Li}$, $n+{}^6\text{Li}^*(3^+; 2.19$ MeV), $d+{}^5\text{He}^*(3/2^-)$
 - $\sim 3,800$ data points; $\chi^2/dof \approx 1.36$
 - formatting changes: MF=4 \rightarrow MF=6; MT=24 \rightarrow 41 (n,2np)

- Updated evaluation (submitted for ENDF/B-VIII.1 β 1)

- upper energy limit $E_n \leq 8.0$ MeV
- new configuration = old config + inelastic: $n_2+{}^6\text{Li}(0^+; 3.56$ MeV)
- new data covering all channels
- corrected ${}^6\text{Li}(n,n'd){}^4\text{He}$ spectra

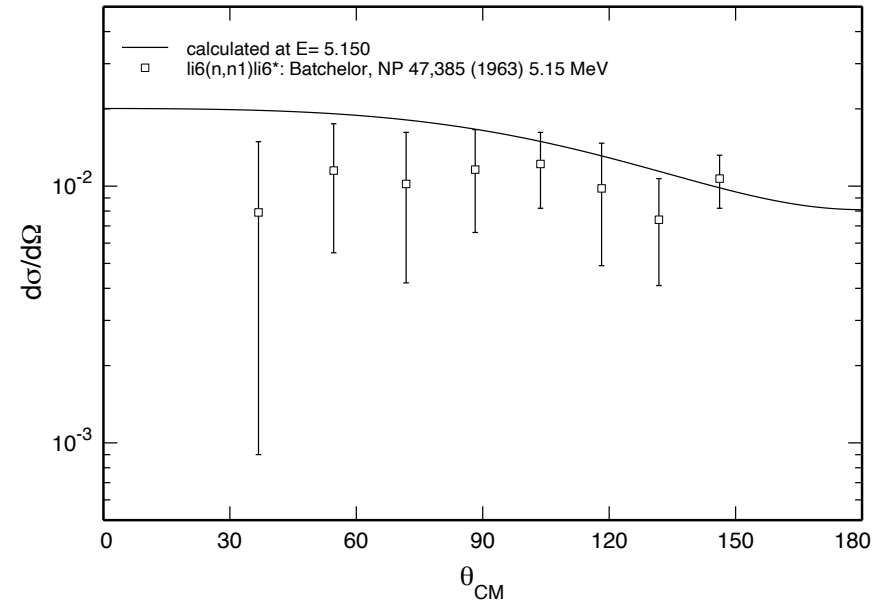


$n+{}^6\text{Li}$

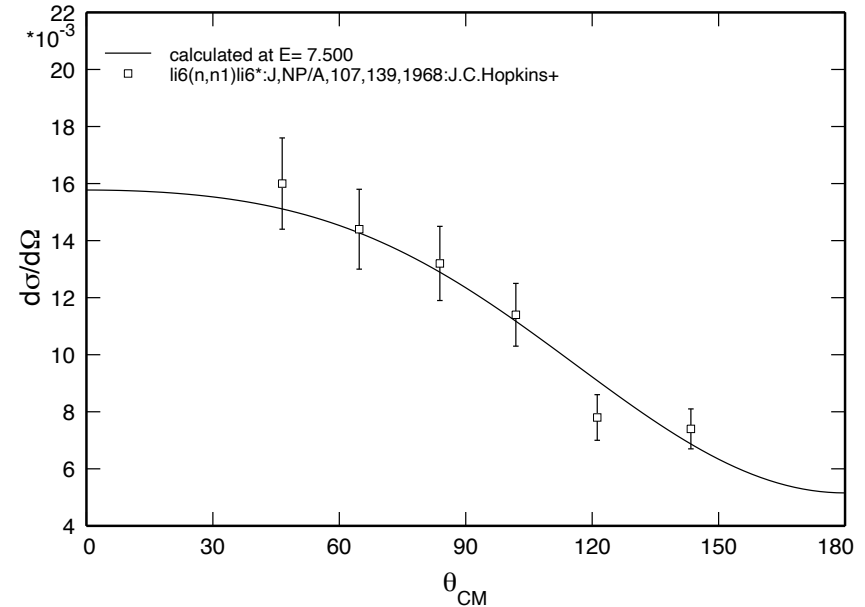
R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VII.1
 - upper energy limit $E_n \leq 4.3$ MeV
 - configuration: $t+{}^4\text{He}$, $n+{}^6\text{Li}$, $n+{}^6\text{Li}^*(3^+; 2.19 \text{ MeV})$, $d+{}^5\text{He}^*(3/2^-)$
 - $\sim 3,800$ data points; $\chi^2/dof \approx 1.36$
 - formatting changes: MF=4 \rightarrow MF=6; MT=24 \rightarrow 41 (n,2np)
- Updated evaluation (submitted for ENDF/B-VIII.1 β 1)
 - upper energy limit $E_n \leq 8.0$ MeV
 - new configuration = old config + inelastic: $n_2+{}^6\text{Li}(0^+; 3.56 \text{ MeV})$
 - new data covering all channels
 - corrected ${}^6\text{Li}(n,n'd){}^4\text{He}$ spectra

$\text{li6}(n,n)\text{li6}^* \text{ d}\sigma/\text{d}\Omega \text{ E= } 5.150 \text{ MeV}$



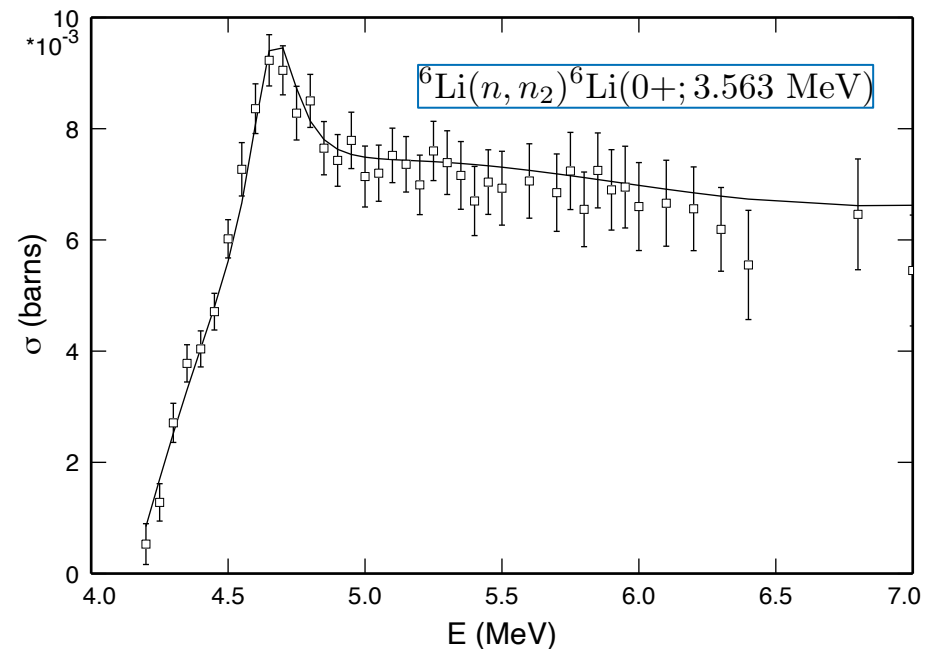
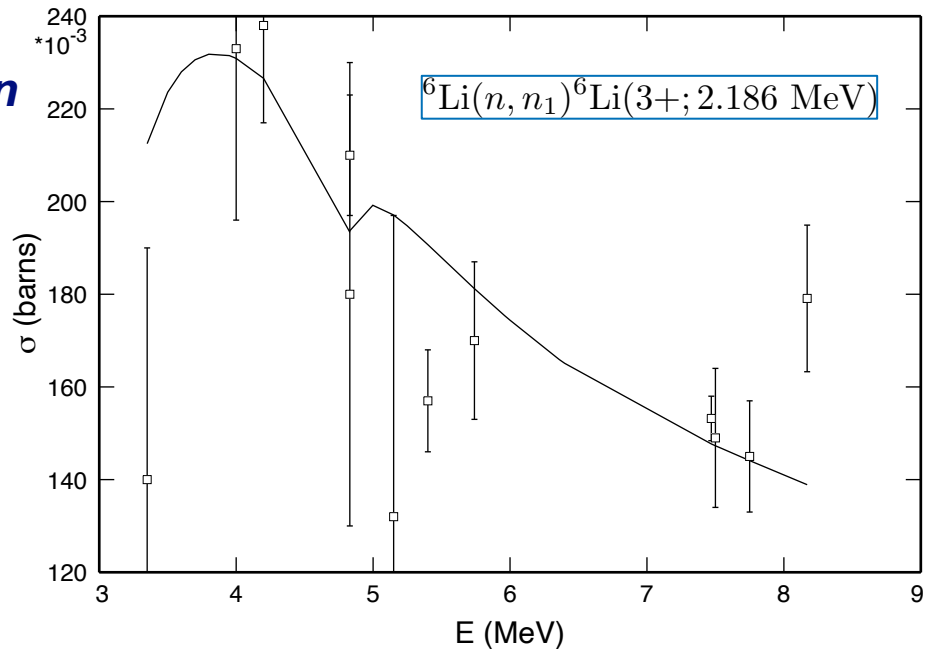
$\text{li6}(n,n)\text{li6}^* \text{ d}\sigma/\text{d}\Omega \text{ E= } 7.500 \text{ MeV}$



$n+{}^6\text{Li}$

R-matrix evaluation update/extension

- Previous evaluation ENDF/B-VII.1
 - upper energy limit $E_n \leq 4.3$ MeV
 - configuration: $t+{}^4\text{He}$, $n+{}^6\text{Li}$, $n+{}^6\text{Li}^*(3^+; 2.19$ MeV), $d+{}^5\text{He}^*(3/2^-)$
 - $\sim 3,800$ data points; $\chi^2/dof \approx 1.36$
 - formatting changes: MF=4 \rightarrow MF=6; MT=24 \rightarrow 41 (n,2np)
- Updated evaluation (submitted for ENDF/B-VIII.1 β 1)
 - upper energy limit $E_n \leq 8.0$ MeV
 - new configuration = old config + inelastic: $n_2+{}^6\text{Li}(0^+; 3.56$ MeV)
 - new data covering all channels
 - corrected ${}^6\text{Li}(n,n'd){}^4\text{He}$ spectra



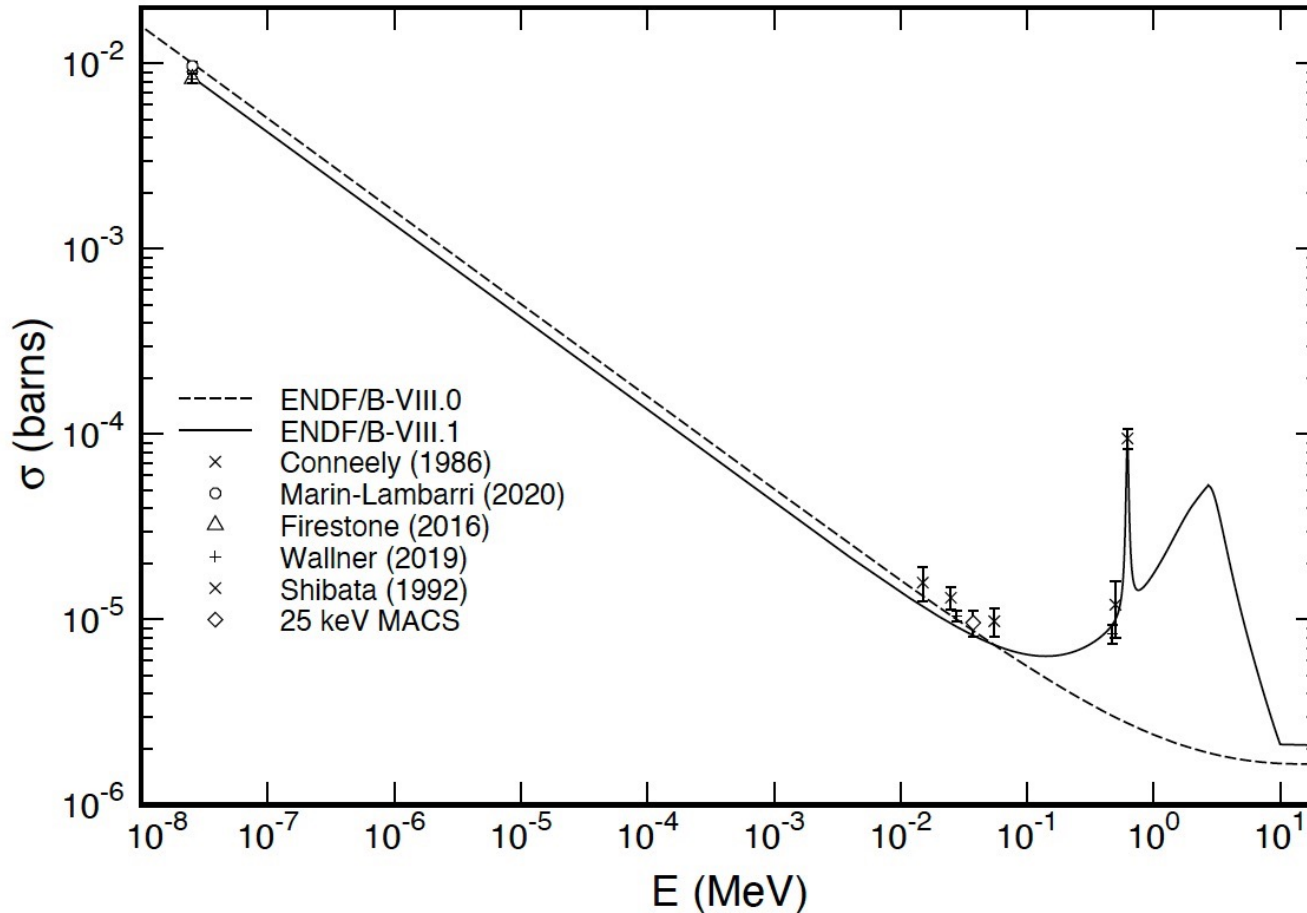
n+⁹Be

R-matrix evaluation update/extension

- New evaluation highlights
 - Added ⁹Be(n,γ)¹⁰Be 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 μ b	3.3 μ b	[76]
30.0 keV	13.00 μ b	1.8 μ b	[76]
55.0 keV	9.79 μ b	1.7 μ b	[76]
27.8 keV	10.44 μ b	0.63 μ b	[78]
473 keV	8.4 μ b	1.0 μ b	[78]
500 keV	12.02 μ b	4.1 μ b	[76]
622 keV	94.80 μ b	12.1 μ b	[76]

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



$n+^{16}\text{O}$

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

- Abbreviated history

- concern that $^{16}\text{O}(n, \alpha)^{13}\text{C}$ absorption in ENDF/B-VIII.0 too large
- LANL/EDA R-matrix fit considers $E_n \leq 7.0$ MeV
- Excited states $E_n > 5.6$ MeV

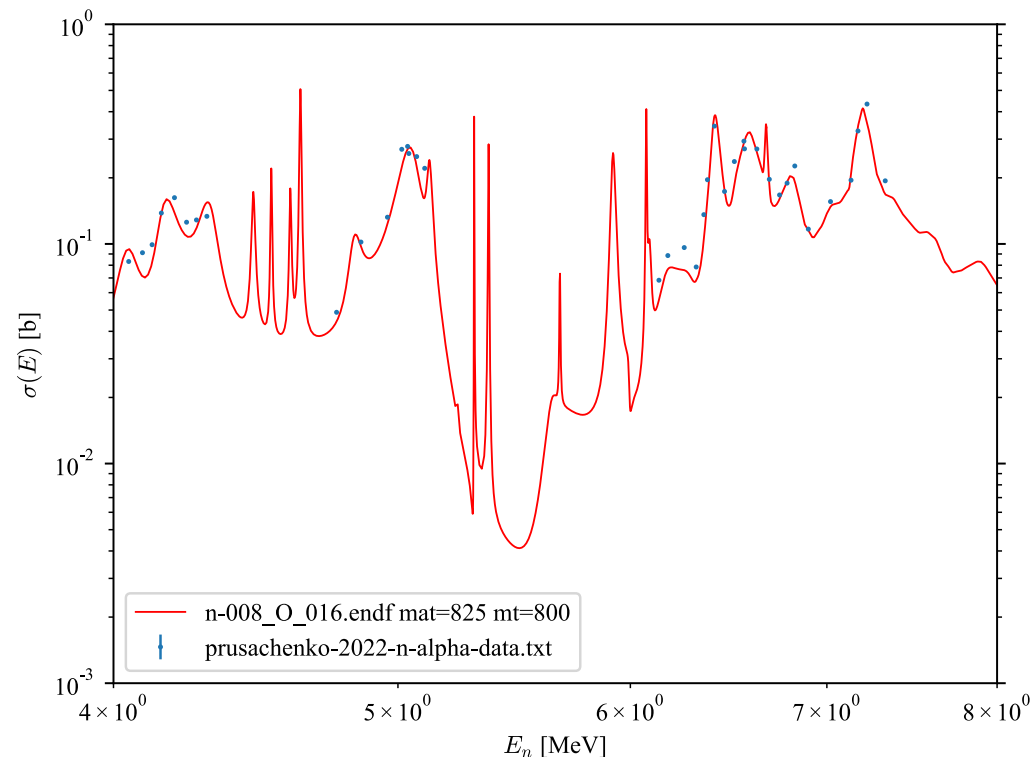
- New data

- 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

$^A Z_i J^\pi$	$E_x(^{13}\text{C})$ (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



$n+^{16}\text{O}$

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

- Abbreviated history

- concern that $^{16}\text{O}(n, \alpha)^{13}\text{C}$ absorption in ENDF/B-VIII.0 too large
- LANL/EDA R-matrix fit considers $E_n \leq 7.0$ MeV
- Excited states $E_n > 5.6$ MeV

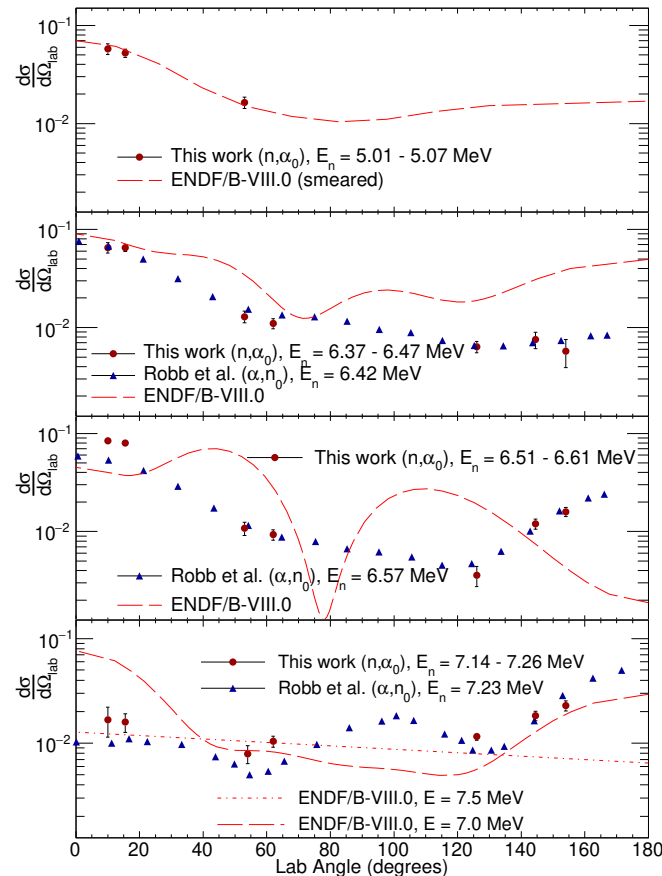
- New data

- supports ENDF/B-VIII.0 to 7.0 MeV
 - Prusachenko et al. IPPE 2022
 - **H.-Y. Lee, S. Kuvin, G. Hale, MP, ...**
– PRC 109, 014601 (2024)

- Implement reduction in (n, α_i)

- $i = 1, 2, 3 \leftrightarrow MT = 801, 802, 803$
- reduced by factor of 2 to agree with Davis

$^A Z_i J^\pi$	$E_x(^{13}\text{C})$ (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



Conclusion

- $n+{}^6\text{Li}$: **Accepted for ENDF/B-VIII.1**
 - reasonably good description of differential data up to 8.0 MeV
- $n+{}^9\text{Be}$: **Accepted for ENDF/B-VIII.1**
 - improved description of capture data
- $n+{}^{16}\text{O}$: **Accepted for ENDF/B-VIII.1**
 - Improved description of (n,α) production data
 - reduced MT=801,802,803 by multiplicative factor of 0.5

- **Aside:**
 - Resonance parameters (MF=2) will not be released for ENDF/B-VIII.1
 - Will be coordinated with new NJOY capabilities for ENDF/B-IX.0

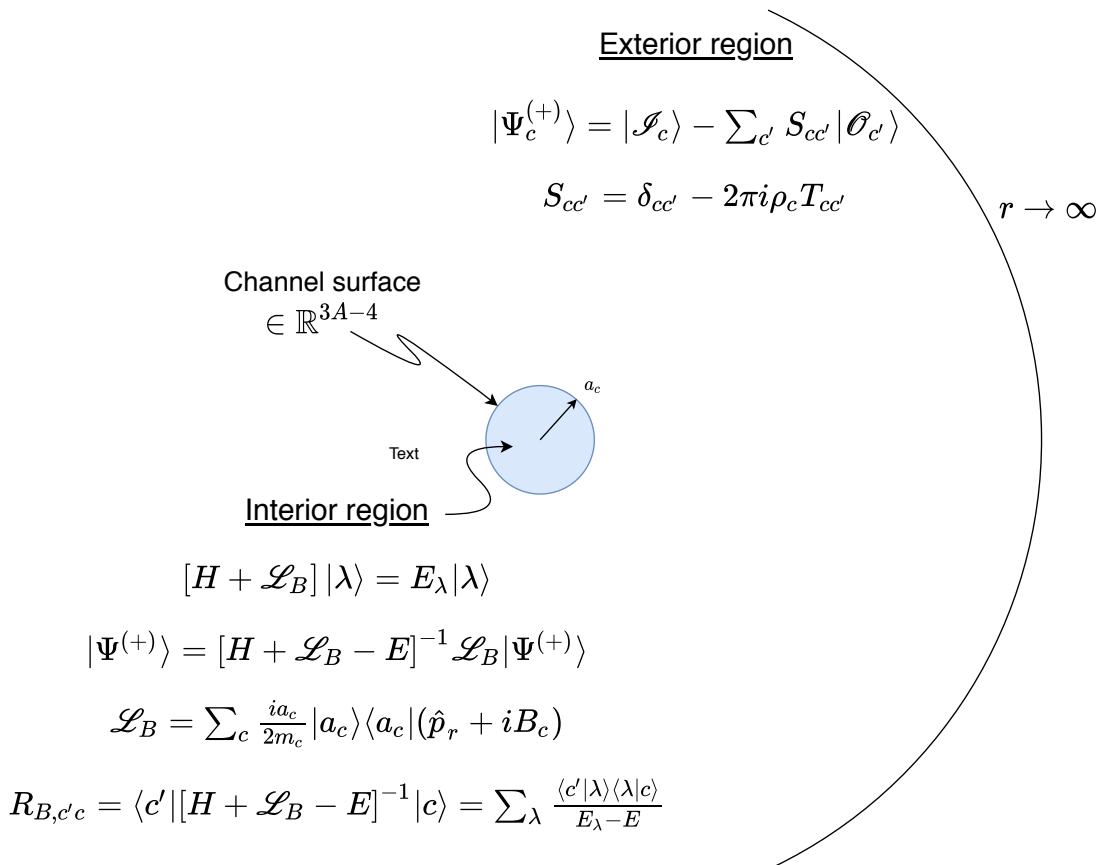


END ENDF END
Thank you!

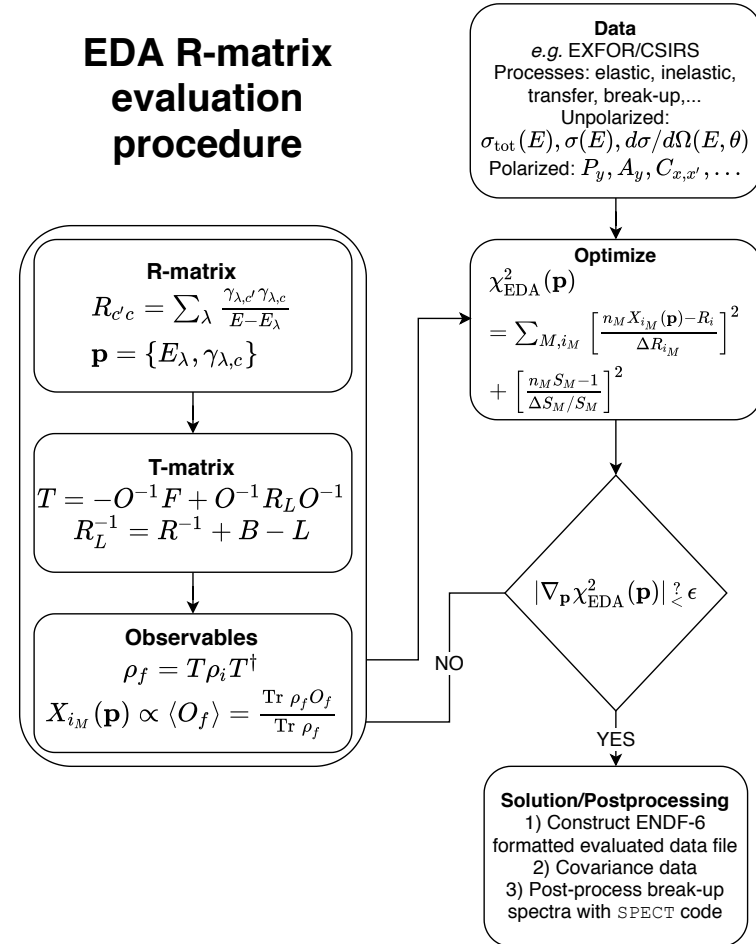


R-matrix

Overview of evaluation framework



EDA R-matrix evaluation procedure



$n+{}^9\text{Be}$

R-matrix configuration

Channel	a_c (fm)	ℓ_{max}
$n+{}^9\text{Be}(\frac{3}{2}^-)$	4.67	3
${}^4\text{He}+{}^6\text{He}(0^+)$	5.00	4
$(nn)_0+{}^8\text{Be}(2^+)$	5.20	3
$n+{}^9\text{Be}^*(\frac{5}{2}^-)$	5.20	1

Process	E_n range	Observables	N_{dat}	χ^2/N_{dat}
${}^9\text{Be}(n, n_0){}^9\text{Be}$	(1.25 eV, 15.4 MeV)	$\sigma_{\text{tot}}, \sigma, \sigma(\theta), A_y(\theta)$	5782	1.65
${}^9\text{Be}(n, {}^4\text{He}){}^6\text{He}$	(0.63, 8.5) MeV	$\sigma, \sigma(\theta)$	178	1.40
${}^9\text{Be}(n, 2n){}^8\text{Be}$	(1.8, 14.7) MeV	σ	40	NA
${}^9\text{Be}(n, n_1){}^9\text{Be}^*$	(2.7, 5.0) MeV	$\sigma(\theta)$	83	1.65
Total			6083	1.75

- Added data: elastic, (n, α) , (n, n_1)
- Extended upper energy from 1.6 MeV to 5.0 MeV

