The Not-So-Short Introduction to Methods of Nuclear Data Evaluations (From Physics to Applications)

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R-matrix School 2025, Oak Ridge National Laboratory
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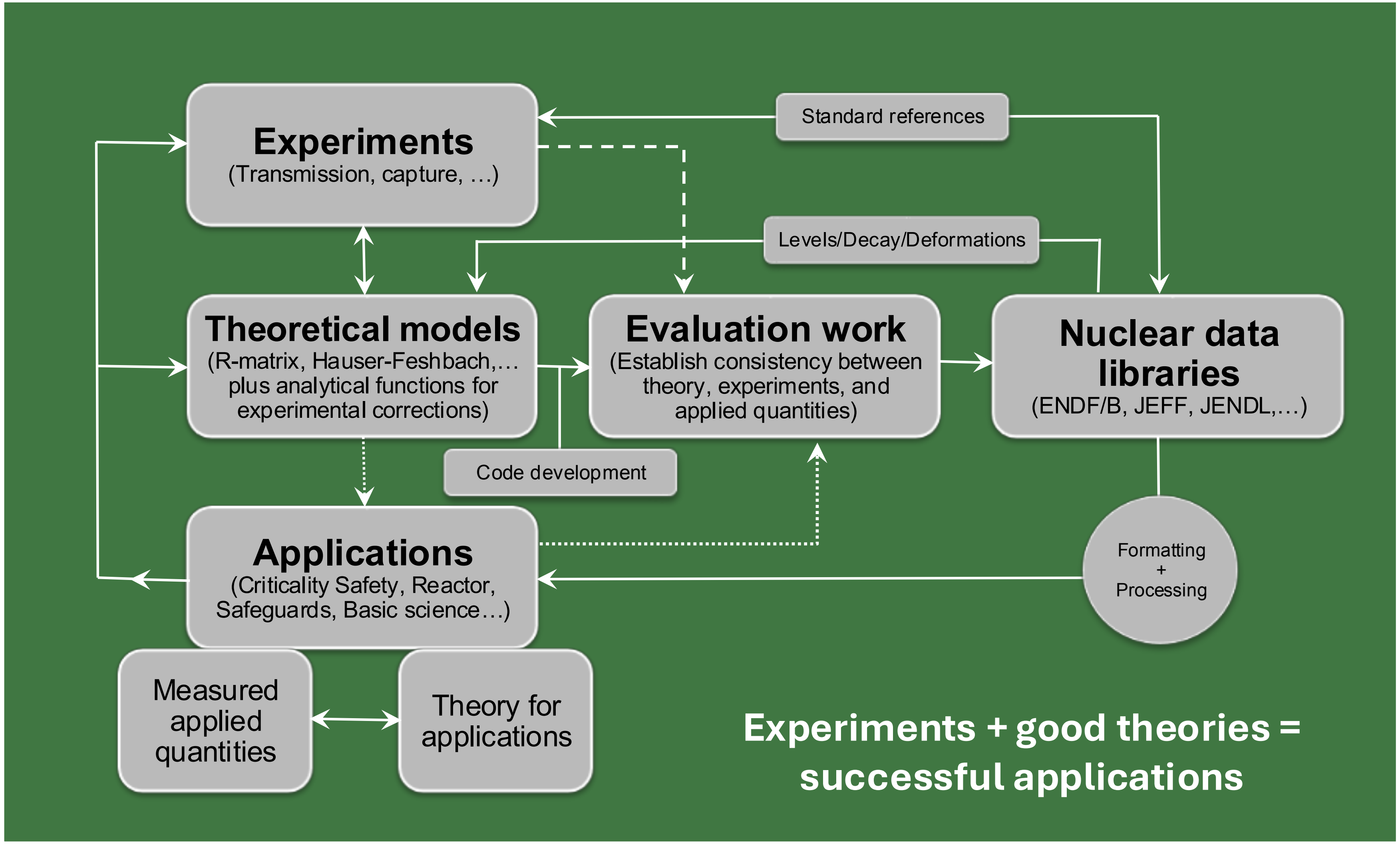
GENERAL WORKFLOW SCHEME



NUCLEAR DATA LIBRARIES @ORNL

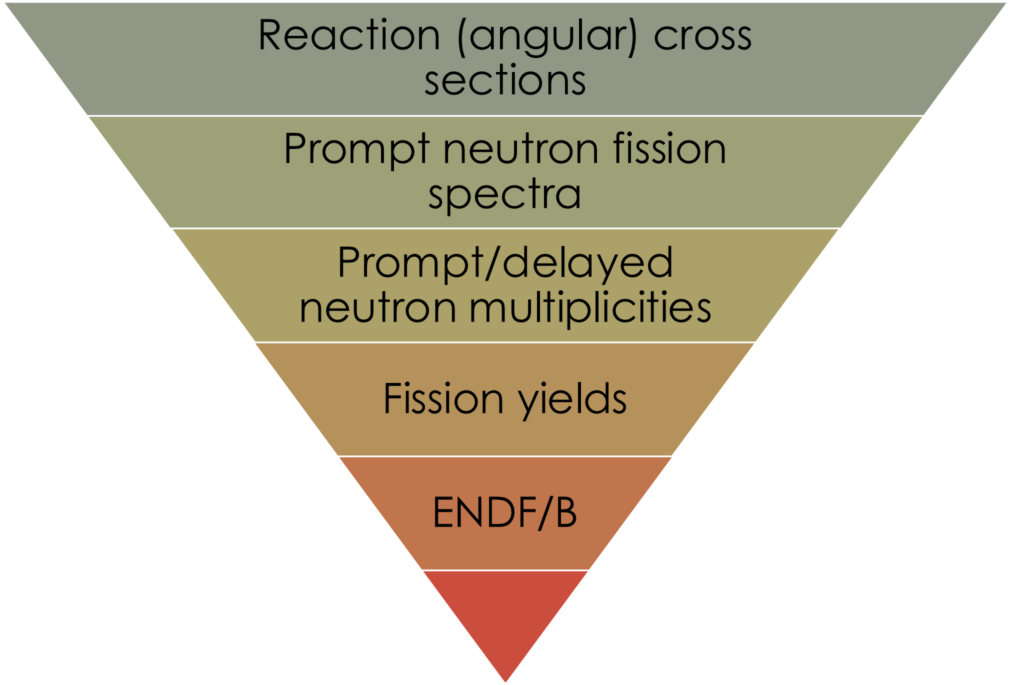
Release of the ENDF/B-VIII.1 nuclear data library (2024)

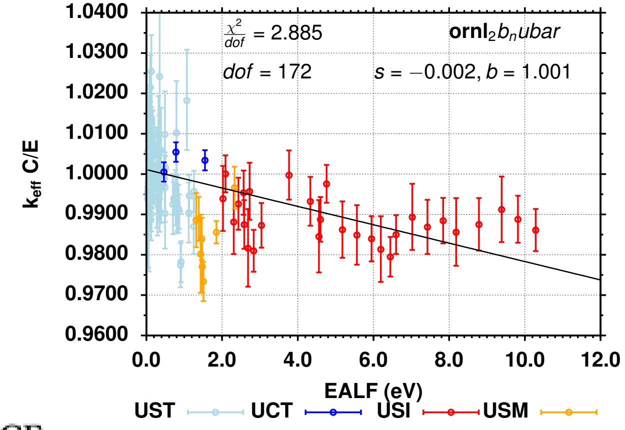
SCALE
- Validation/benchmarks
- Processing

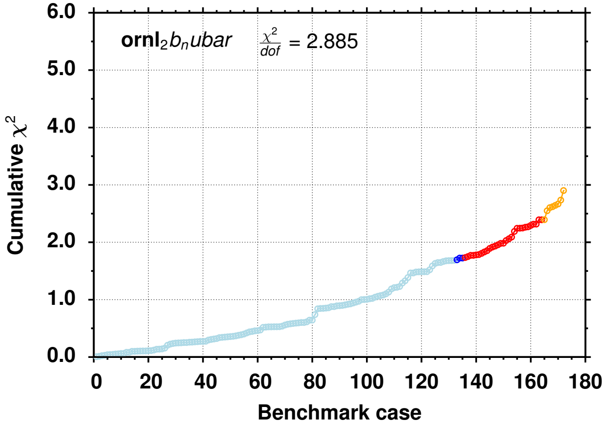
Evaluation
- Theory
- Experiments
- Uncertainty quantification

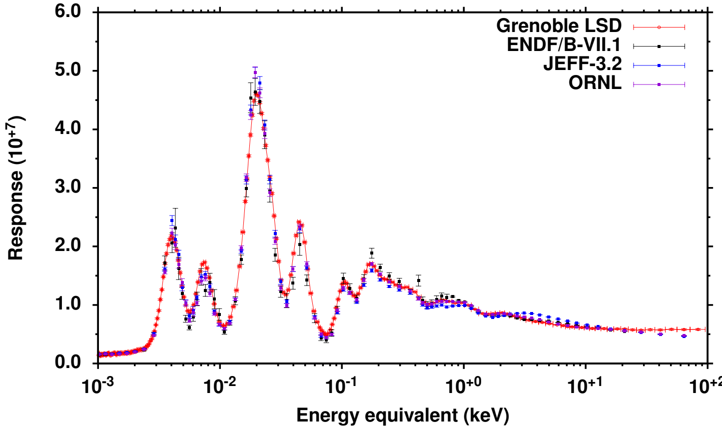
SAMMY
- Computing
- Modeling

NUCLEAR DATA LIBRARY VALIDATION

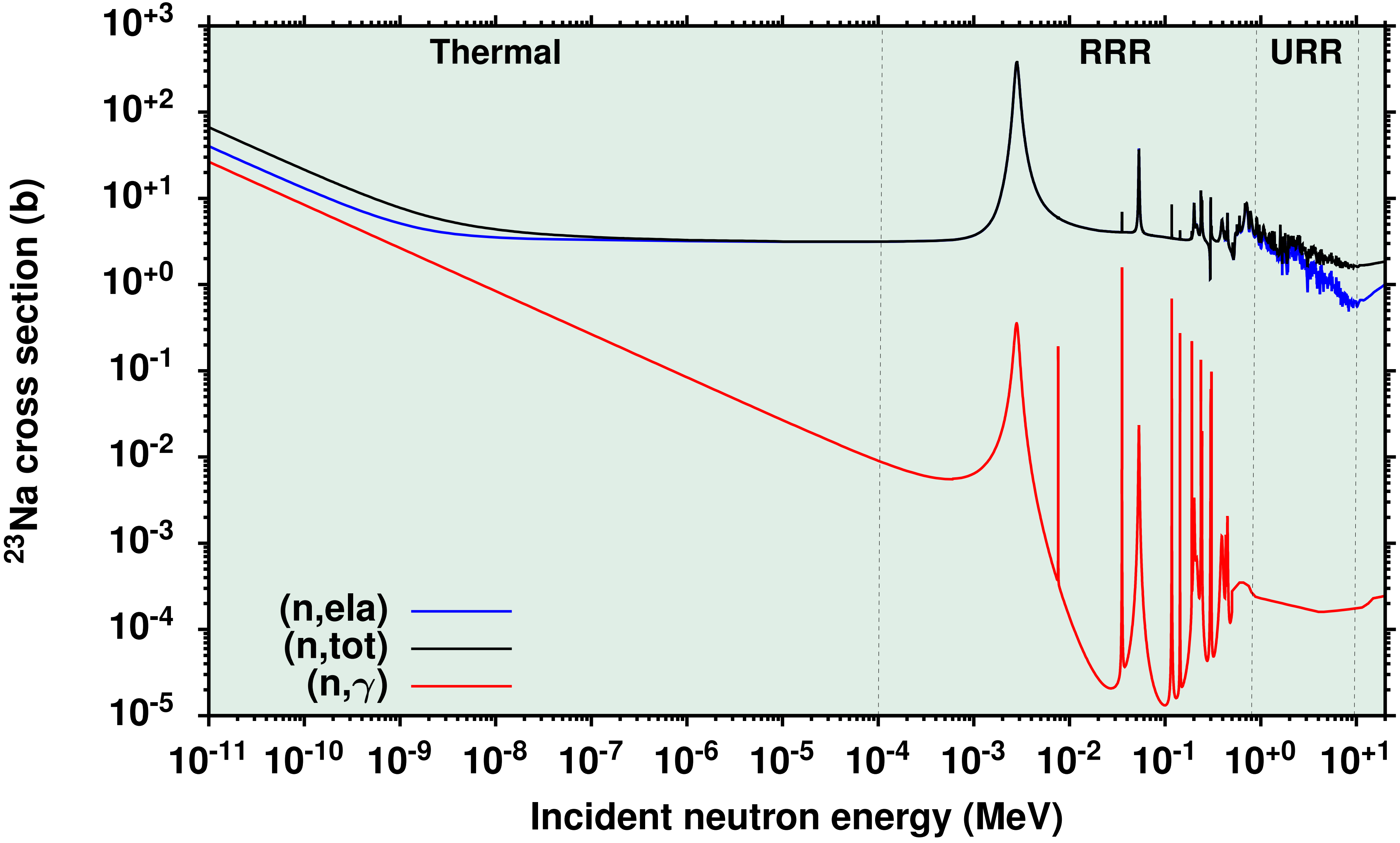




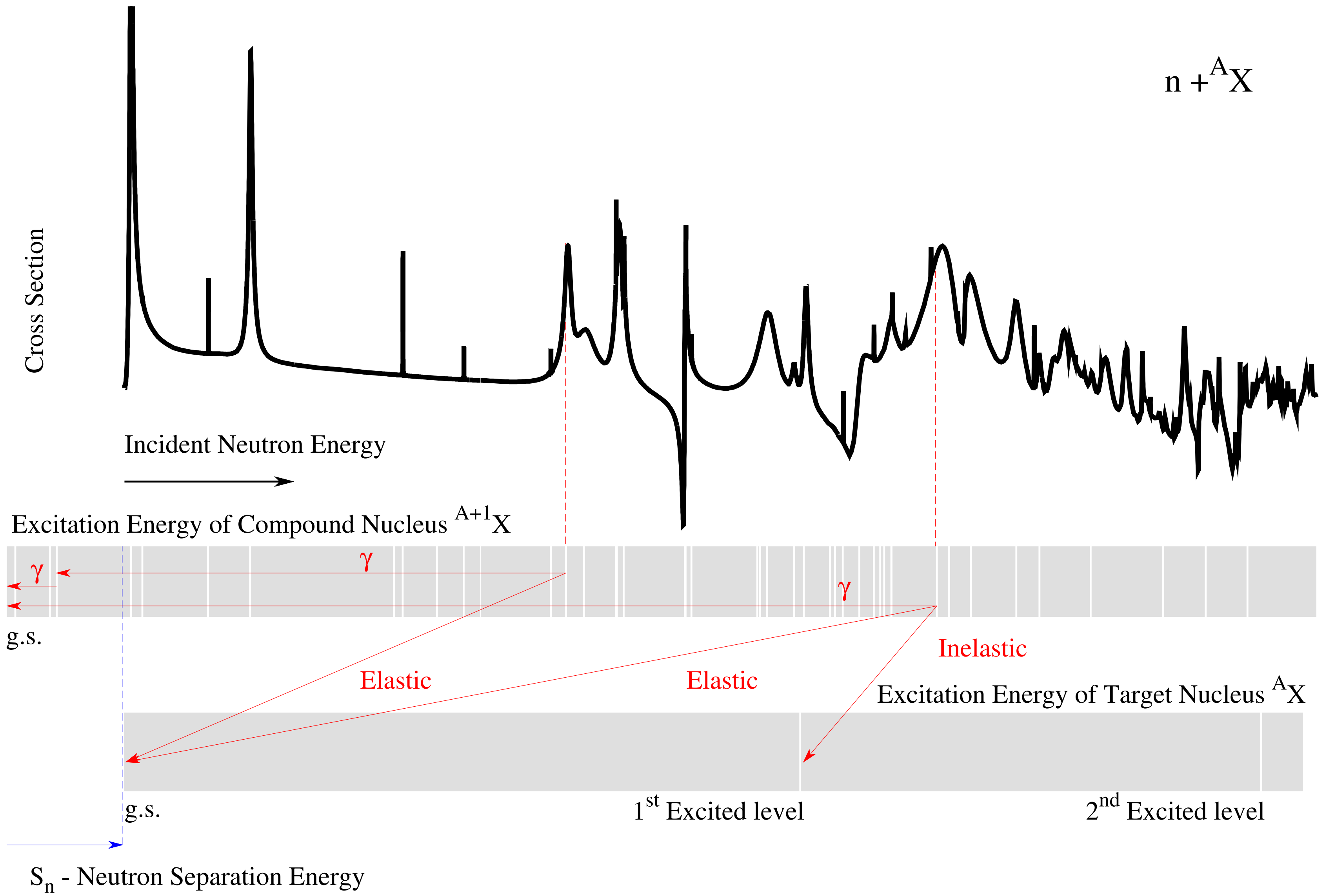




NUCLEAR EVALUATED DATA



RESONANCES AND RESONANCE PARAMETERS



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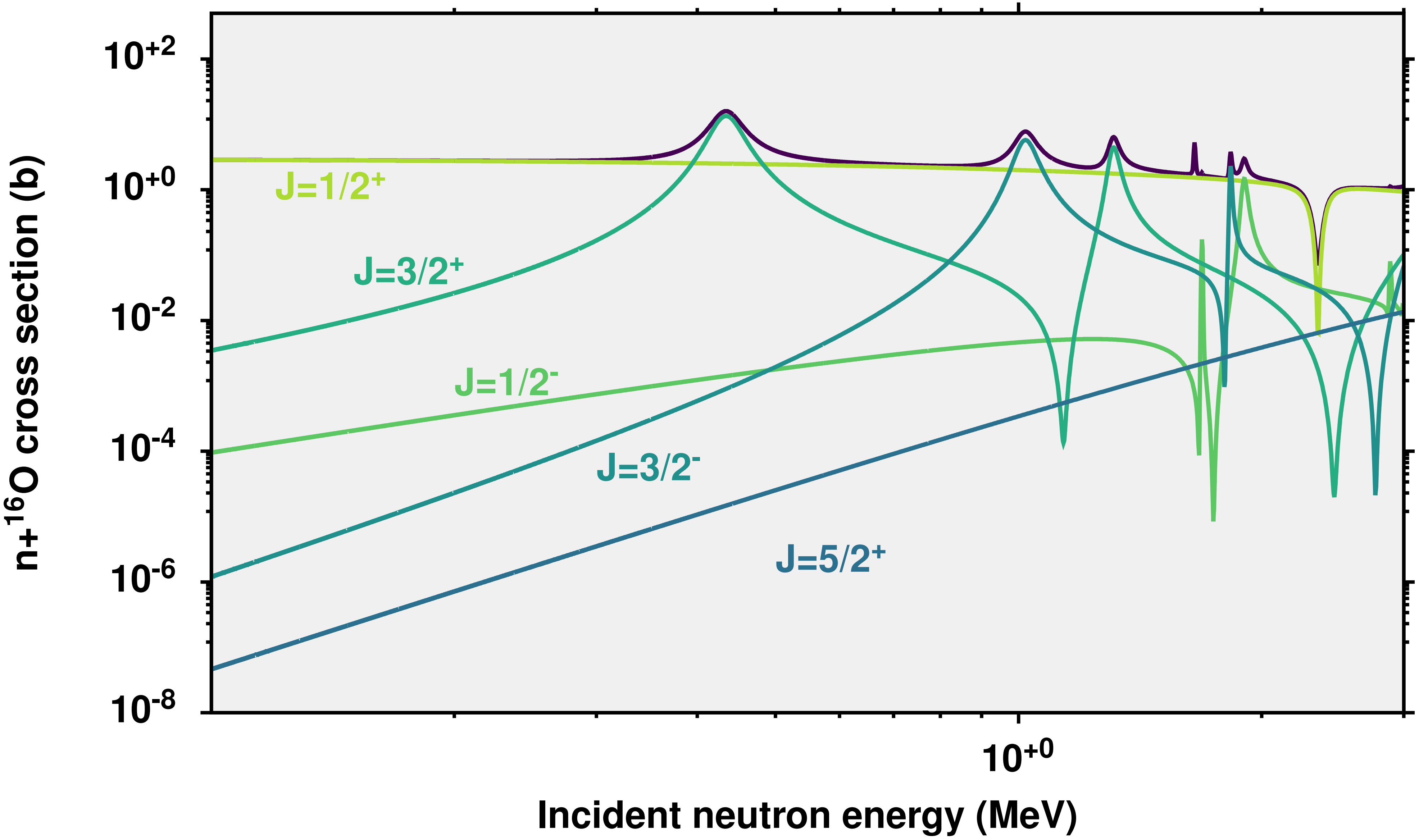

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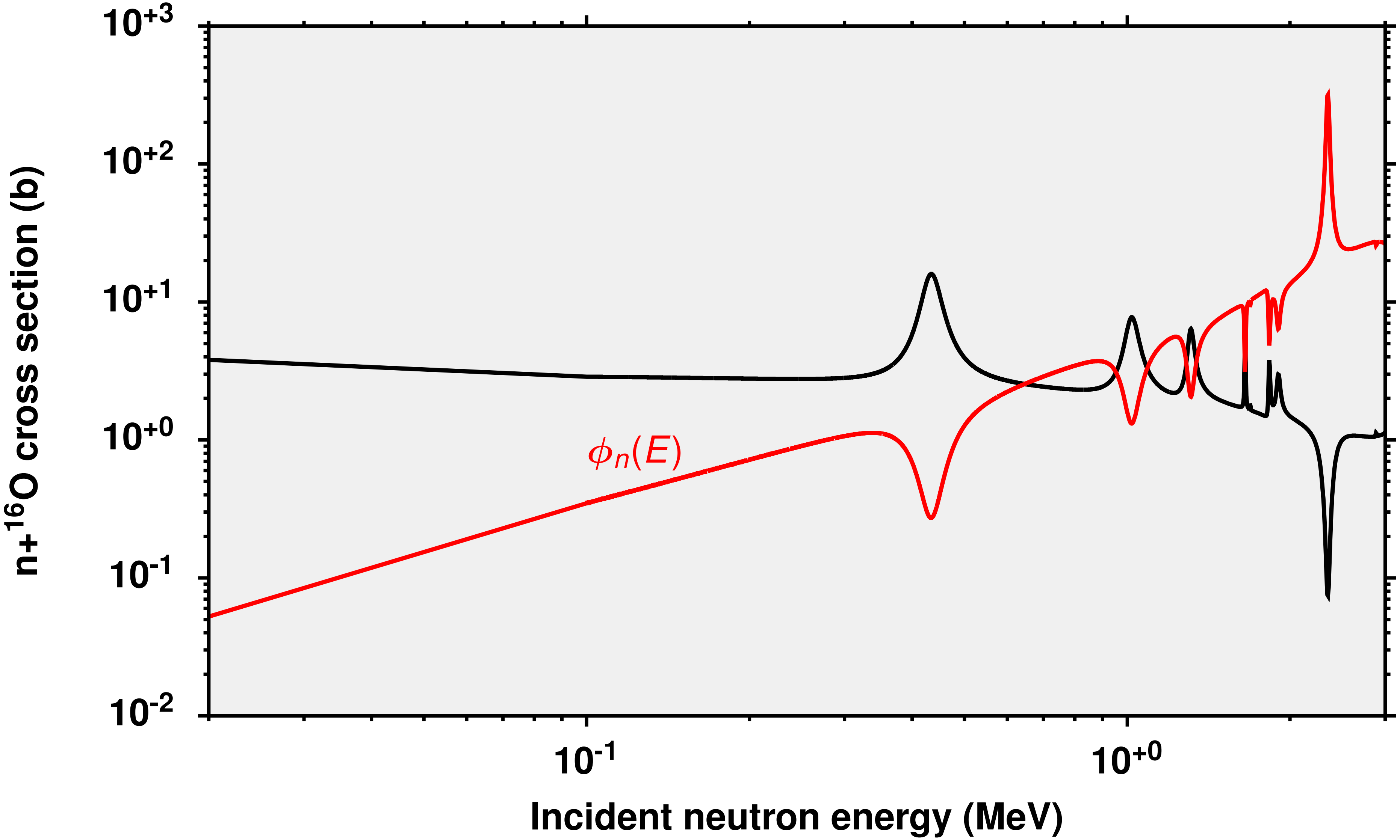

RESONANCES AND RESONANCE PARAMETERS

Newly Evaluated Neutron Reaction Data on Chromium Isotopes

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R. Arcilla,[1] J. Gutierrez,[5] A. Cuadra,[6] G. Arbanas,[2] B. Kos,[4] D. Bernard,[7] and P. Leconte[7]

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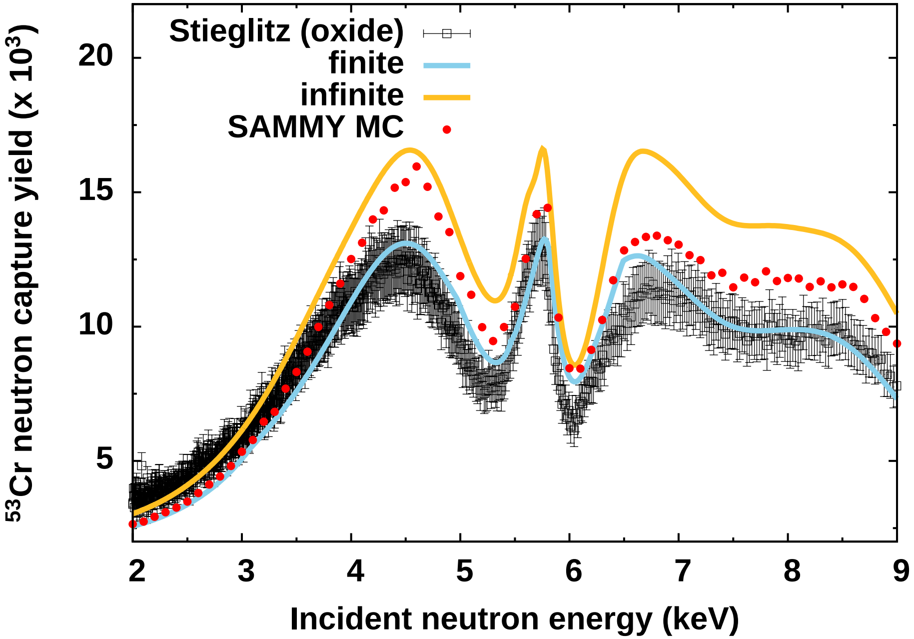
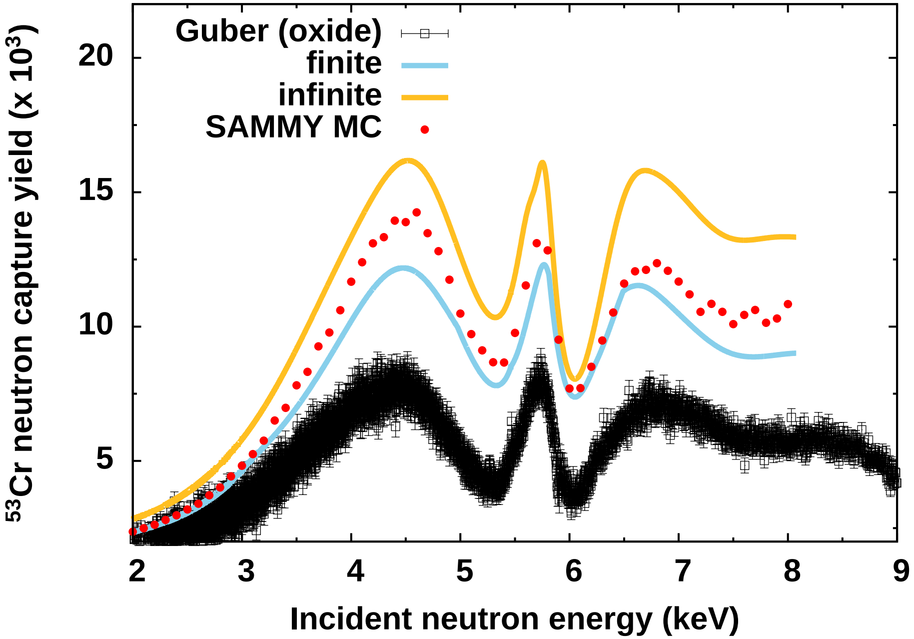
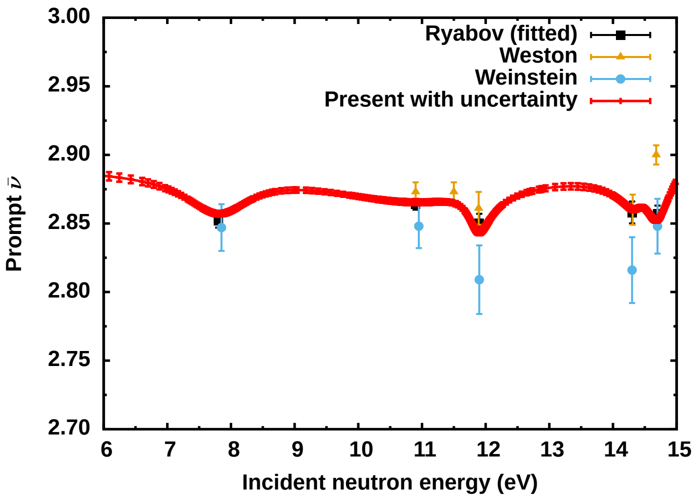
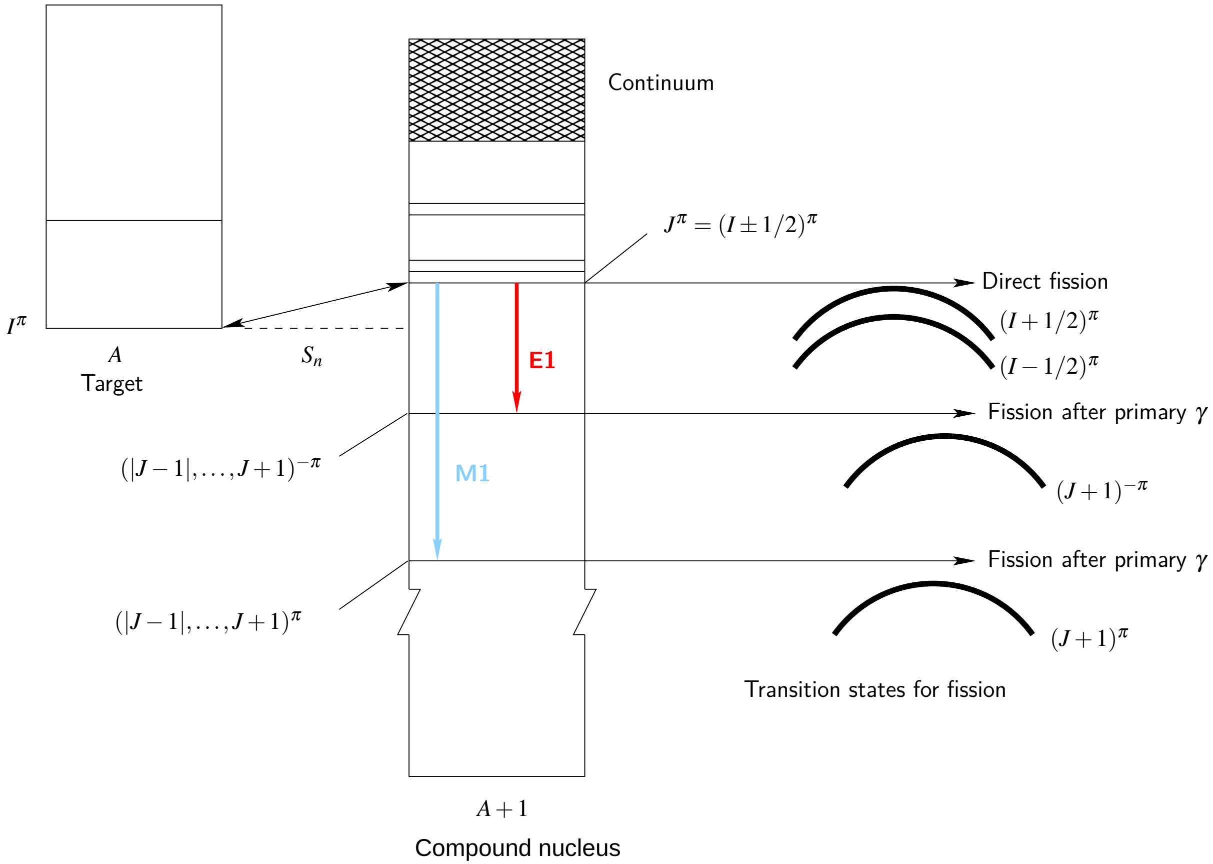
(Dated: December 11, 2020)





NEUTRON MULTIPLICITIES OF ^{239}Pu

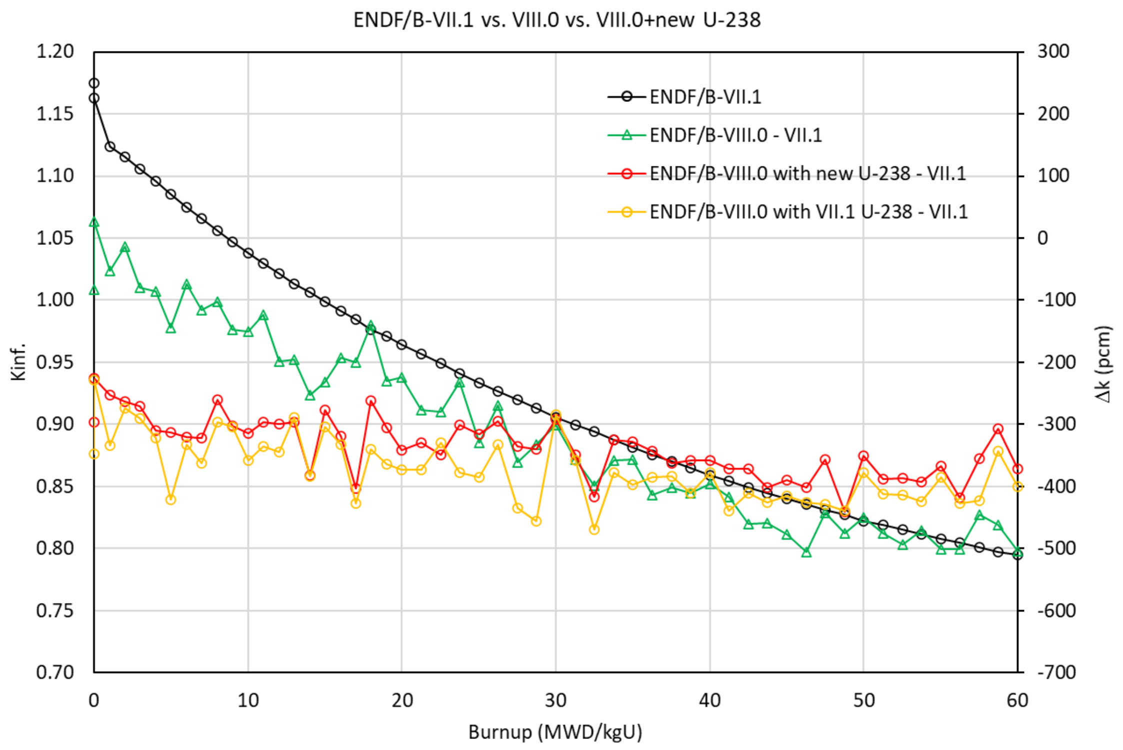


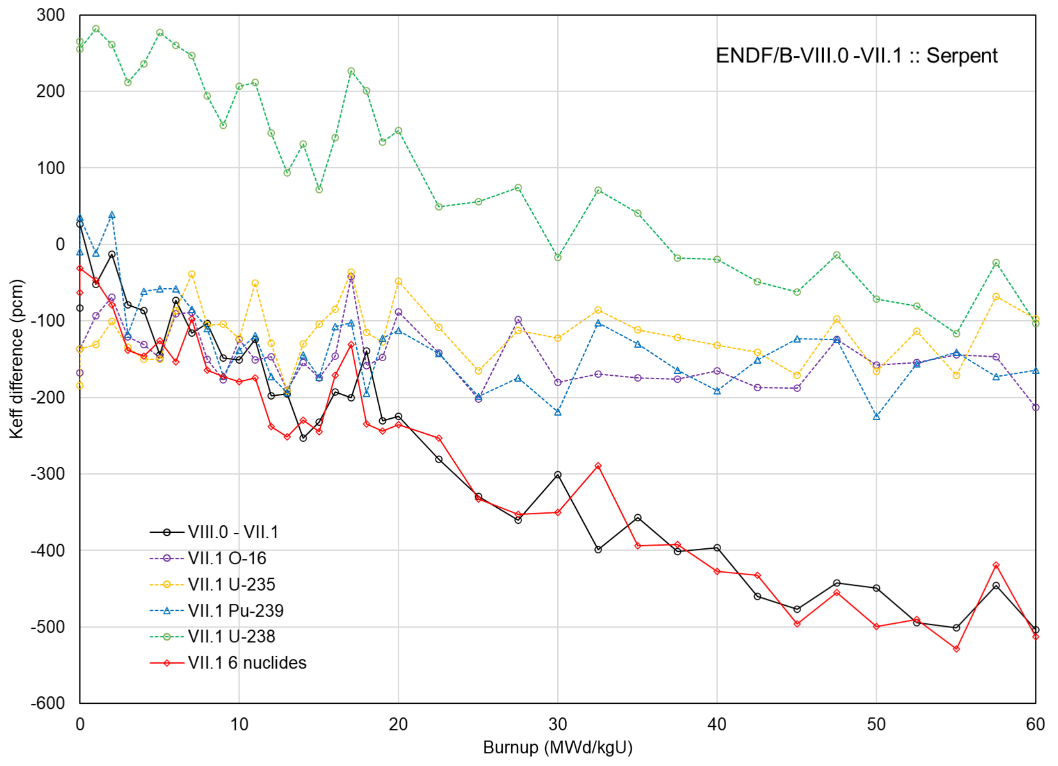


- Prompt neutron multiplicities $\bar{\nu}_{\mathrm{p}}$ have a large impact on criticality
- Fluctuating behaviour linked to $(\mathrm{n},\gamma\mathrm{f})$ process
- Poorly described measured data

DEPLETION VS CRITICALITY

- Focus on resolving reactivity rates in VERA benchmark results[1]
- Four nuclides, i.e. ^{239}Pu, ^{235,238}U, and ^{16}O, contribute to the low reactivity at high burnup points[2]





[1]Kang Seog Kim et al., CSEWG2019
[2]Calculations performed by Kang Seog Kim.

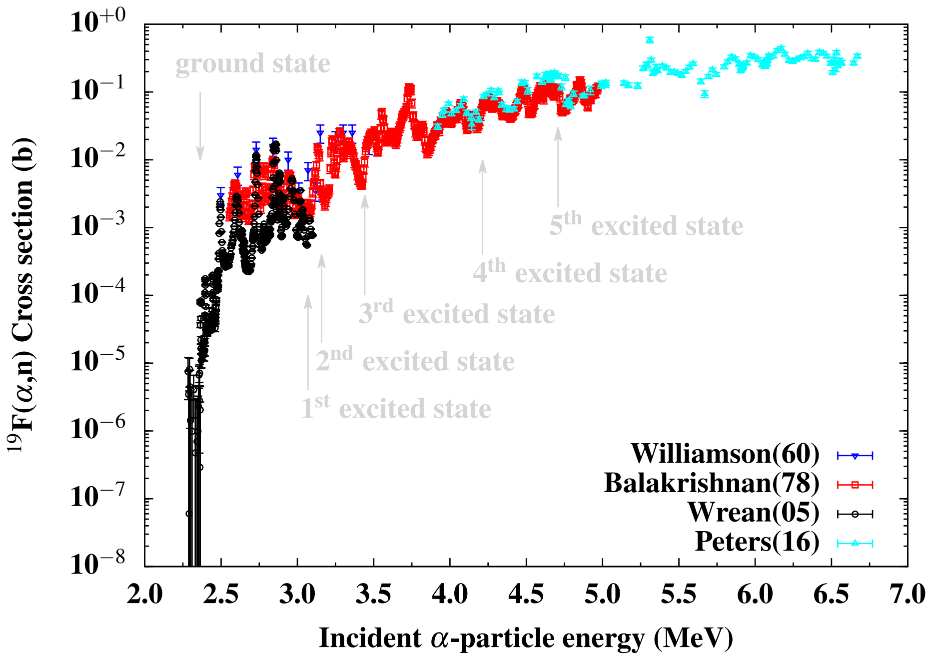
CHARGED-PARTICLE LIBRARIES

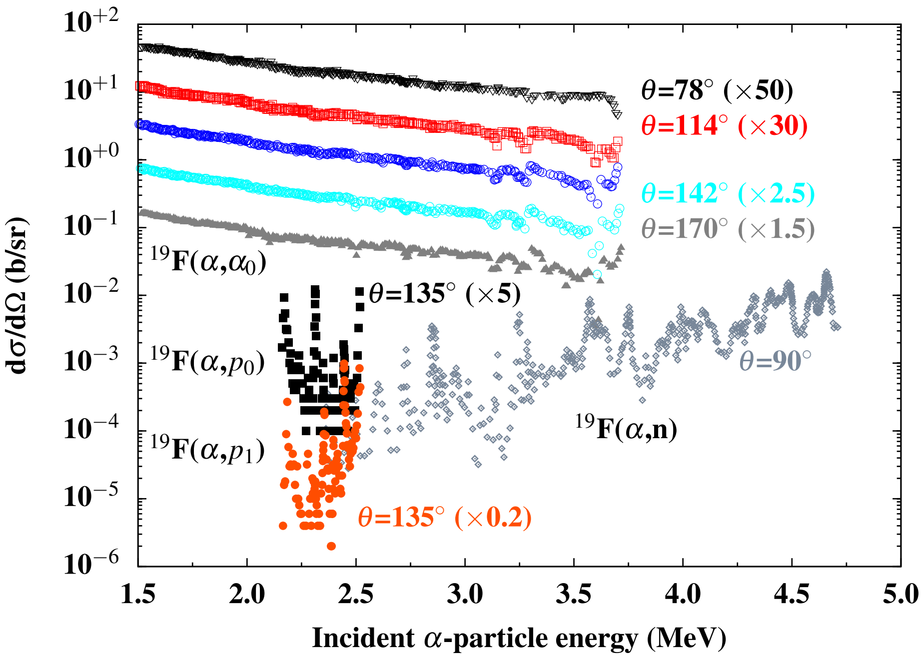
Neutron source term Y_n from (α,n) reactions

- (α,n) reaction cross-sections

$$Y_\mathrm{n} \propto \sum_i \int_0^{E\alpha} \sigma_i(E)\,\varepsilon(E)^{-1} dE$$

- Stopping power cross sections





CHARGED-PARTICLE LIBRARIES (ENDF φ-1)

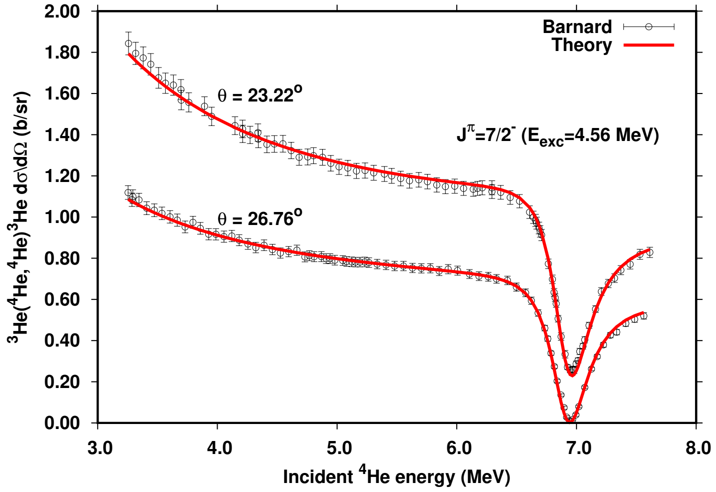
Library Type	Total ENDF	Nucleus (MAT)	E_{max} (MeV)	MF	MT	Source
deuteron≡^{2}H	6	^{2}H (128)	20	3/6	2/50/600	LLNL
		^{3}H (131)	20	3/6	2/50/51/91	LLNL
				12/14/15	91	
		^{3}He (225)	20	3/6	2/600	LANL
		^{4}He (228)	10	3	2/28	LANL
				6	2	
		^{6}Li (325)	20	3/6	2/50/600/800	LANL
		^{7}Li (328)	20	3/6	2/16/22/103/700	LLNL

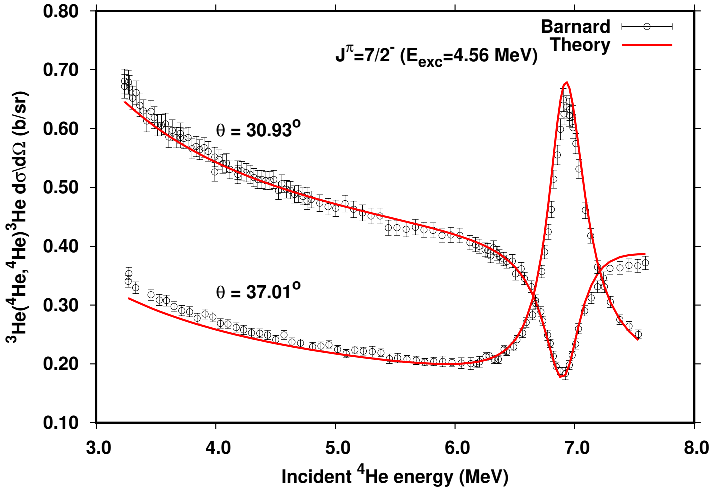
Library Type	Total ENDF	Nucleus (MAT)	E_{max} (MeV)	MF	MT	Source
triton≡^{3}H	5	^{3}H (131)	20	3/6	2/16	LLNL
		^{3}He (225)	20	3/6	2/28/650	LANL
		^{4}He (228)	20	3/6	2	LLNL
		^{6}Li (325)	20	3/6	2/16/50/600/650	LANL
		^{7}Li (328)	20	3/6	2/17/24/50	LLNL

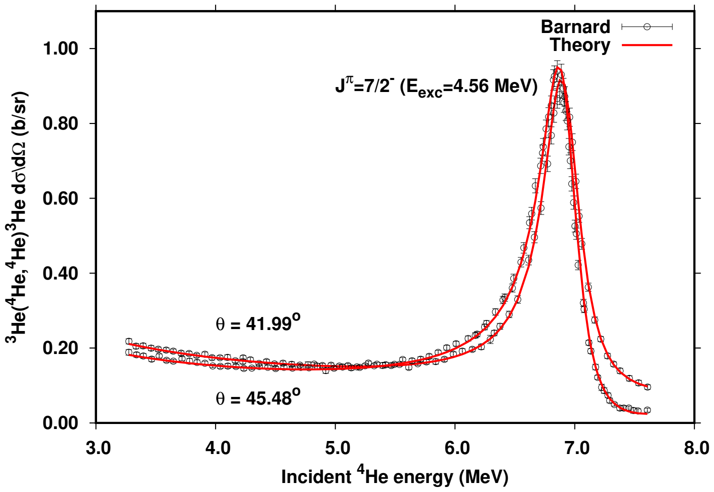
Library Type	Total ENDF	Nucleus (MAT)	E_{max} (MeV)	MF	MT	Source
helium≡^{3}He	4	^{3}He (225)	20	3/6	2/111	LLNL
		^{4}He (228)	20	2/3/6	2/600	LLNL
		^{6}Li (325)	20	3/6	104/112	LLNL
		^{7}Li (328)	20	3/6	45/105/117/600/800/802	LLNL
				12/14	802	

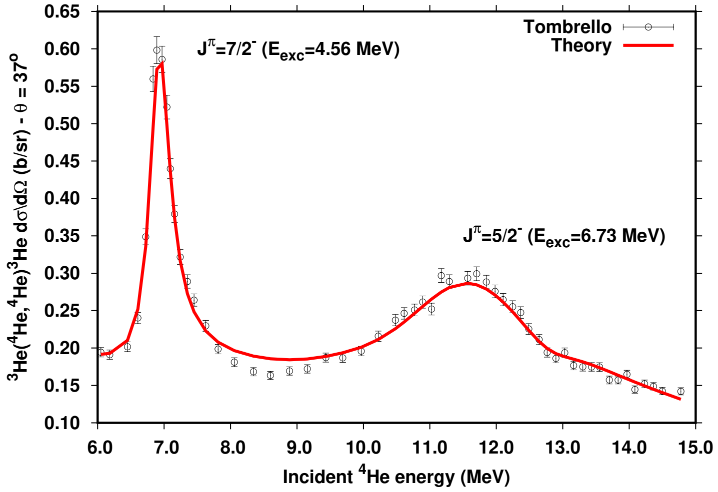
Library Type	Total ENDF	Nucleus (MAT)	E_{max} (MeV)	MF	MT	Source
alpha≡^{4}He	5	^{4}He (228)	20	3/6	2	LANL
		^{6}Li (325)	20	3/6	600/650/651	LLNL
		^{9}Be (425)	15	3	2/4/22/50–52/91/201	NNL
				6	2/22/50-52/91	
		^{17}O (828)	15	3	2/4/22/50–53/91/201	NNL
				6	2/22/50–53/91	
		^{18}O (831)	15	3	2/4/16/22/50–54/91/201	NNL
				6	2/16/22/50–54/91	

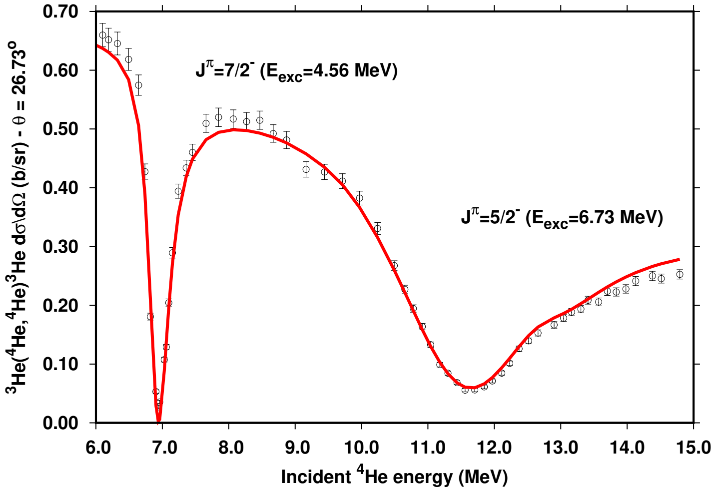
$^3He(^4He,^4He)^3He$ RESULTS (preliminary)

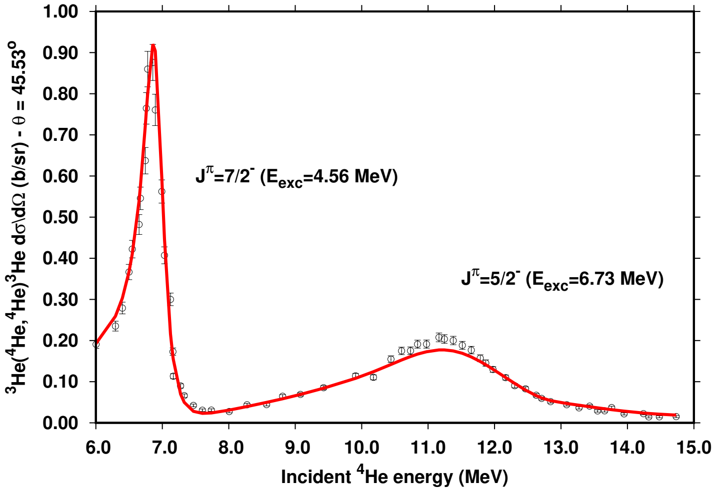




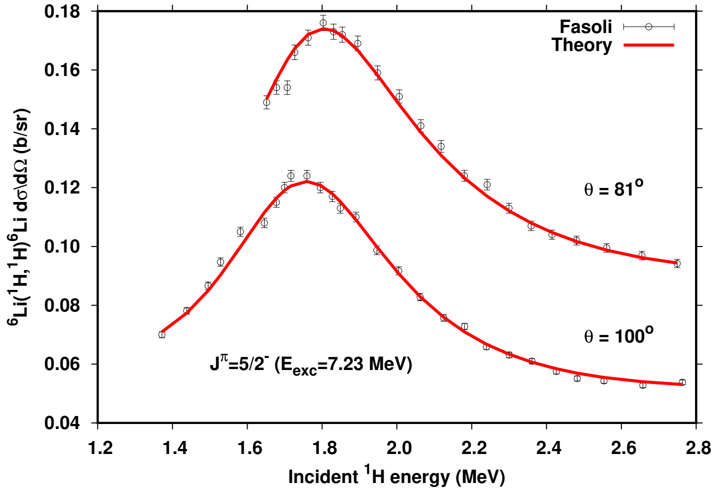


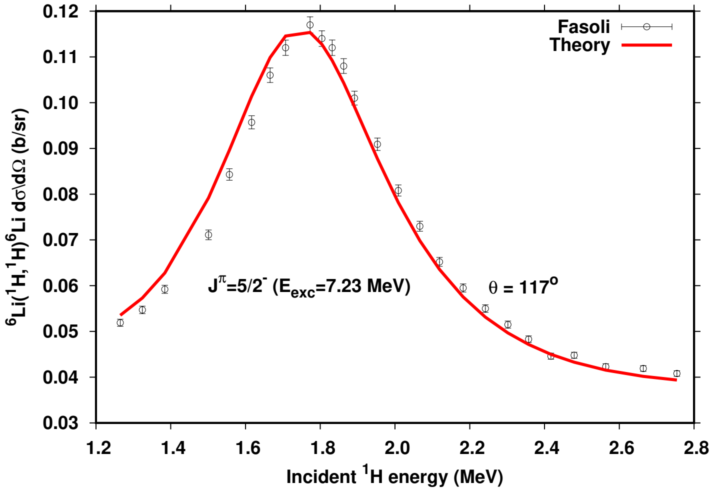


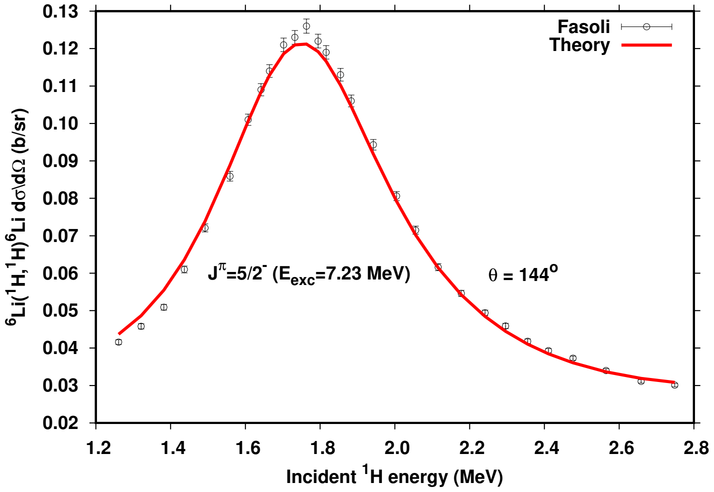


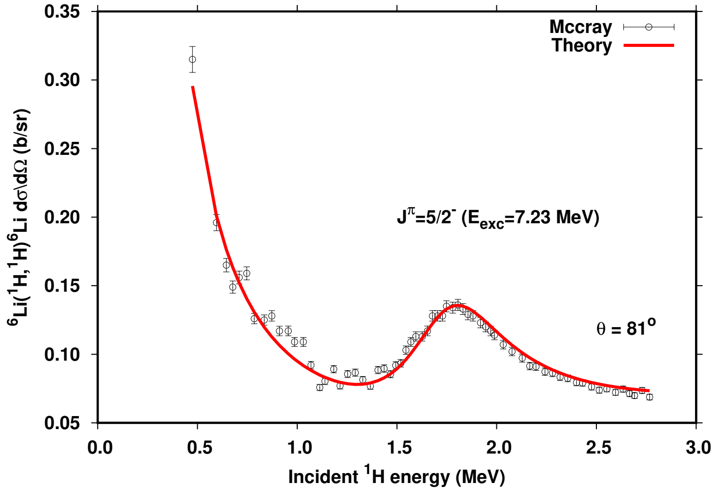


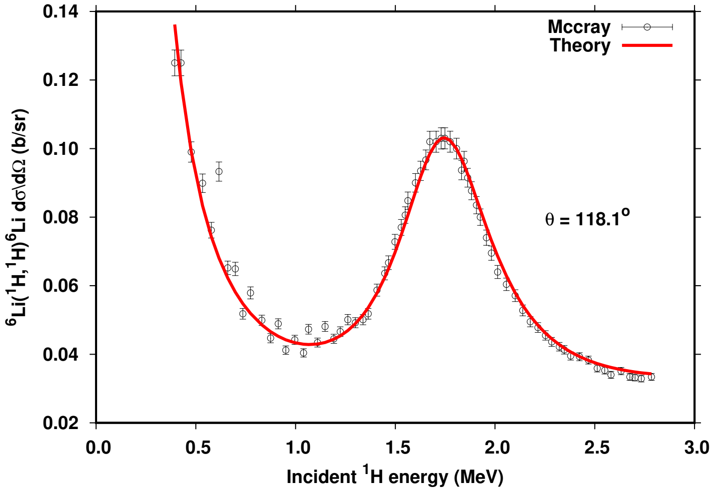
$^{6}Li(^{1}H,^{1}H)^{6}Li$ RESULTS (preliminary)

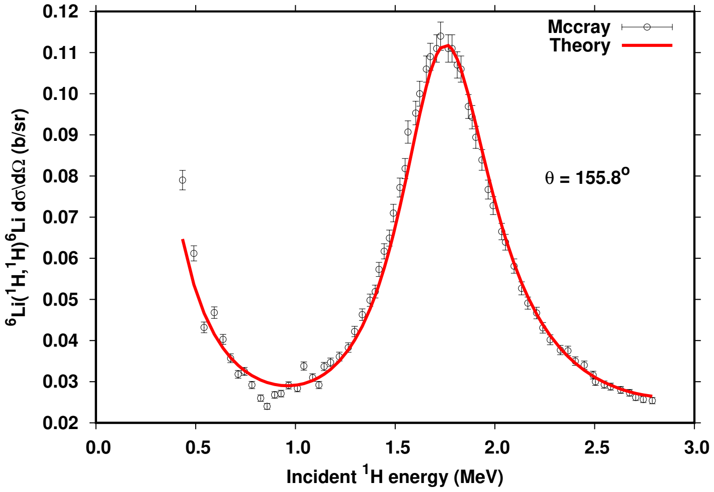












APPENDIX : R-MATRIX ALGORITHM

- For the incident c and exit channel c'
- The angle-integrated reaction cross section $c \to c'$

$$\sigma_{cc'}(E) = \frac{\pi}{k_c^2} \sum_J g_J \sum_c |\delta_{cc'} - \mathsf{U}^J_{cc'}(E)|^2 ,$$

- The collision matrix $\mathsf{U}^J_{cc'}$ in terms of the level matrix $\mathsf{A}_{\lambda\mu}$

$$\mathsf{U}^J_{cc'}(E) = \Omega_c(E;a_c)\left[\delta_{cc'} + 2\imath\sqrt{P_c(E;a_c)} \sum_{\lambda\mu} \gamma_{\lambda(c,J)} \mathsf{A}_{\lambda\mu} \gamma_{\mu(c',J)} \sqrt{P_{c'}(E;a_{c'})}\right] \Omega_{c'}(E;a_{c'}) ,$$

$$\mathsf{A}^{-1}_{\lambda\mu} = (E_\lambda - E)\delta_{\lambda\mu} - \Delta_{\lambda\mu} - \frac{\imath}{2}\Gamma_{\lambda\mu} ,$$

- Shift factor functions S_c, the boundary conditions B_c, and the reduced-width amplitudes γ_λ, γ_μ

$$\Delta_{\lambda\mu}(E) = \sum_c \gamma_{\lambda(c,J)} [S_c(E;a_c) - B_c] \gamma_{\mu(c,J)}$$

$$\Gamma_{\lambda\mu}(E) = 2 \sum_c \gamma_{\lambda(c,J)} P_c(E;a_c) \gamma_{\mu(c,J)}$$

APPENDIX: PRE-EQUILIBRIUM AND HAUSER-FESHBACH

- Interval $[0,\tau]$ for PE emission (exciton model) and $[\tau,\infty)$ for compound nucleus (CN) emission[3]
- In multistep HF calculations containing both pre-compound and compound effects

$$\sigma_{cc'}(E;\varepsilon_{c'})d\varepsilon_{c'} = \left(\frac{\lambda_c^2}{4\pi}\right)\sum_{J\pi sl} g_J \mathsf{T}^J_{cls}(\varepsilon_{c'})\frac{d\varepsilon_{c'}}{D_{J\pi}}\sum_{s'l'}\mathsf{T}^J_{c'l's'}(\varepsilon_{c'})\omega_{c'}(I,E,U) \tag{1}$$

where

$$\omega_c(I,E,U) = \sum_p \mathrm{C}_c(p,E)\rho_c(p-1,h,I,U)$$

- $\mathsf{T}^J_{cls} = 1-|\mathsf{S}^J_{cls}|^2$: transmission coefficient (optical model)
- $\omega_c \equiv \rho_c(I,U)$, Eq. (1) reduces to the usual HF formula for instantaneous equilibration ($\tau \rightarrow 0$)

$$\sigma_{cc'}(E;\varepsilon_{c'})d\varepsilon_{c'} = \left(\frac{\lambda_{c'}^2}{4\pi}\right)\sum_{J\pi lsl's'} g_J \frac{\mathsf{T}^J_{cls}\mathsf{T}^J_{c'l's'}}{D_{J\pi}}\rho_{c'}(I,U)d\varepsilon_{c'} \tag{2}$$

[3] TNG-GENOA ORNL/TM-2000/252 ENDF-363

APPENDIX : n+^{239}Pu(n,γf) (two-step process) reaction

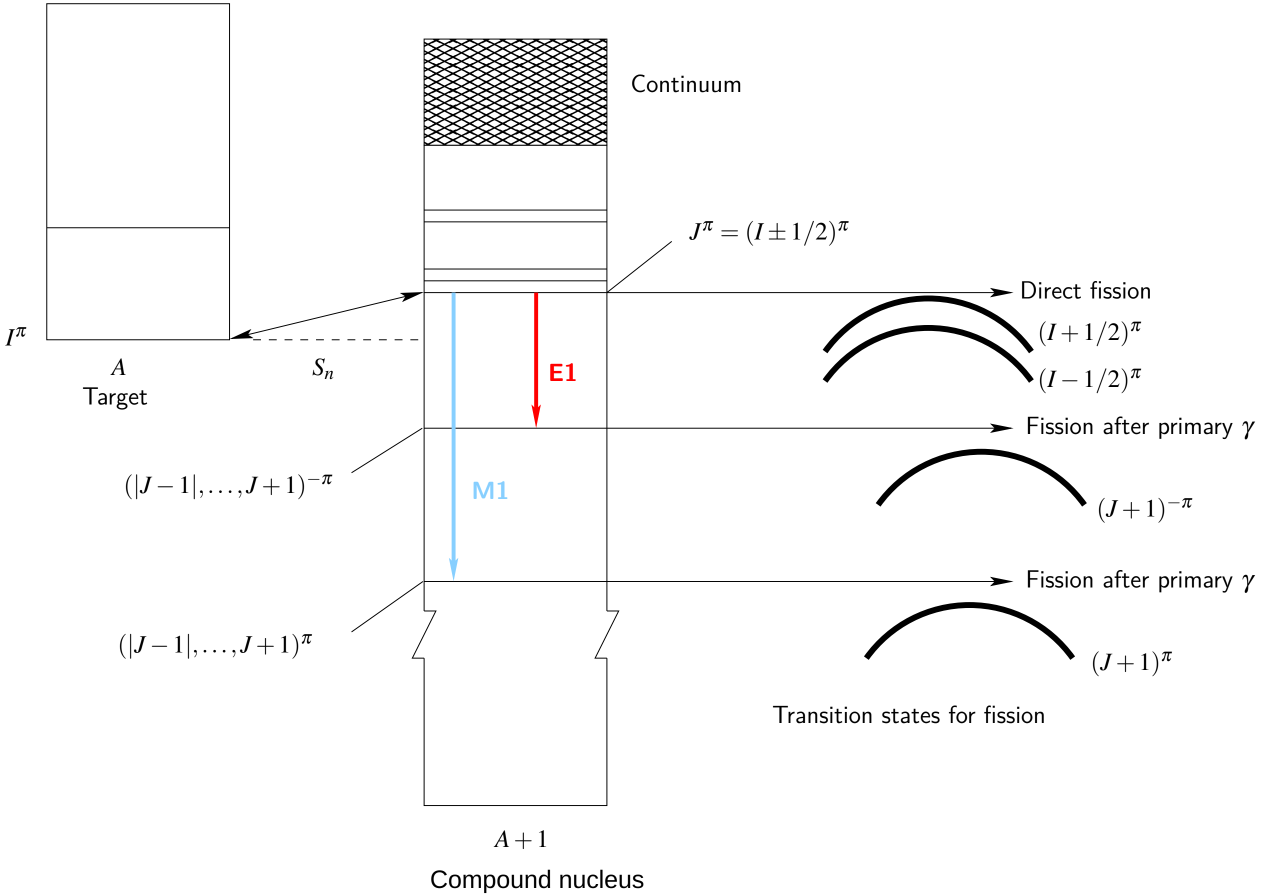


Figure 1: Schematic diagram of the (n,γf) reaction (Lynn 1965). After the emission of a primary γ-ray (e.g. E1, M1,..), the compound nucleus may still be in a highly excited state that may decay by fission as an alternative to secondary γ-ray emission. In the two-stage decay, the compound nucleus can be in an intermediate state that differs from the initial state depending on the multi-polarity of the transition.

APPENDIX : α+^{17,18}O evaluations (applied observables)

- Anderson et al., measured the energy-dependent neutron spectrum from (α,n) reactions and spontaneous fission performed within a series of measurements from a moderated and unmoderated ^{238}Pu–^{18}O source with enriched ^{18}O (e.g., up to 31%), which made the neutron spectra dominated by the (α,n) reaction component

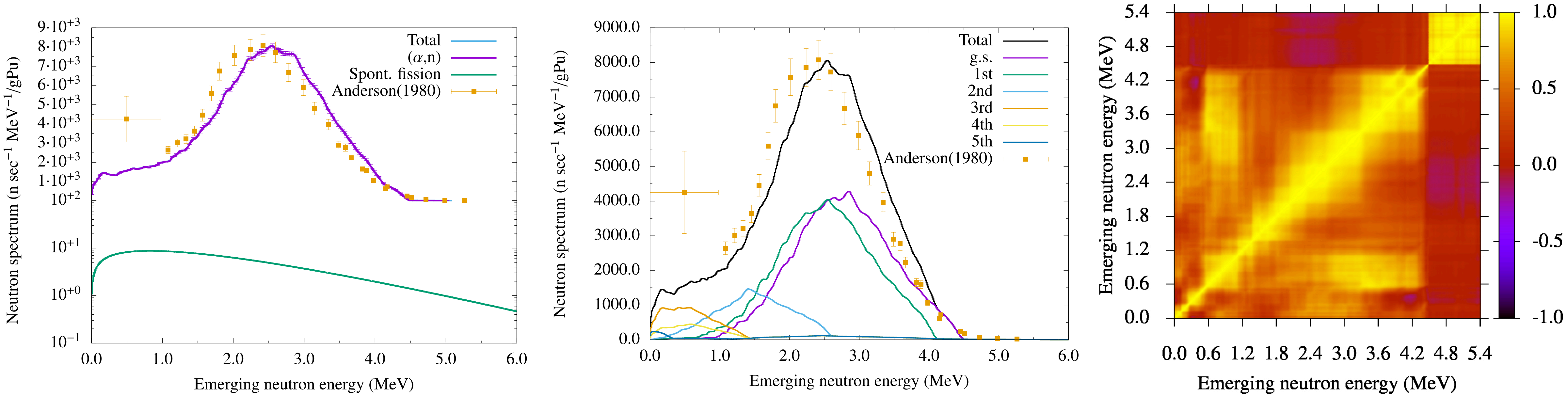


Figure 2: Total (left) and partial (right) neutron energy spectrum calculated by ORIGEN code (SOURCES4C methods). The partial contributions related to spontaneous fission and (α,n) reactions are also shown together with measured data. Neutron spectra covariance matrix is shown on the right.

ACKNOWLEDGMENTS

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