EDA R-matrix evaluations for light-elements

Nuclear Data Week/CSEWG

Evaluations session

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Motivation & Outline

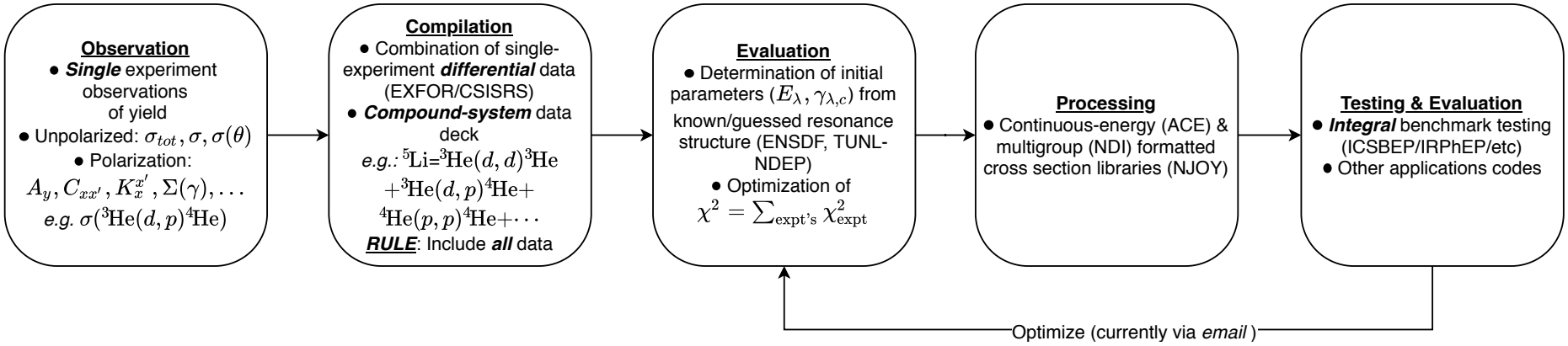
- ***Updating evaluation sublibraries***
  - **Neutron:** `n-001_H_001.endf,n-003_Li_006.endf,n-004_Be_009.endf`
  - **Proton:** `p-001_H_001.endf,p-002_He_004.endf`
  - **Deuteron:** `d-002_He_003.endf`
  - **Triton:** `t-002_He_004.endf`
- ***Motivation:*** improve fidelity of charged-particle and n-induced evaluations
- ***Validation:*** IAEA; NJOY; pencil-beam; quasi-int. (Danon); Faust (Herman)

- **EDA** evaluation pipeline
  - Overview/reminder
- *High-fidelity, unitary* **R-matrix** approach
  - Simultaneous evaluation of ***all*** data
- Evaluation reproduction
  - Challenges in push-button/script-driven reproducibility for our approach

NB: our evaluation approach is currently heavily hand-spun
  - Automation *limited* but *under development*

Overview
Light-element evaluation

Nuclear Data Pipeline
EDA cross section evaluation



- Data-cull: observables from single experiments are compiled
- Evaluation: one set of variational parameters for all data
  - Unitary parametrization: highly constraining between different processes
    - Elastic & reaction cross sections are coupled in complex ways
  - Not simply drawing smooth curves
- Processing/Verfication/Validation

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

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

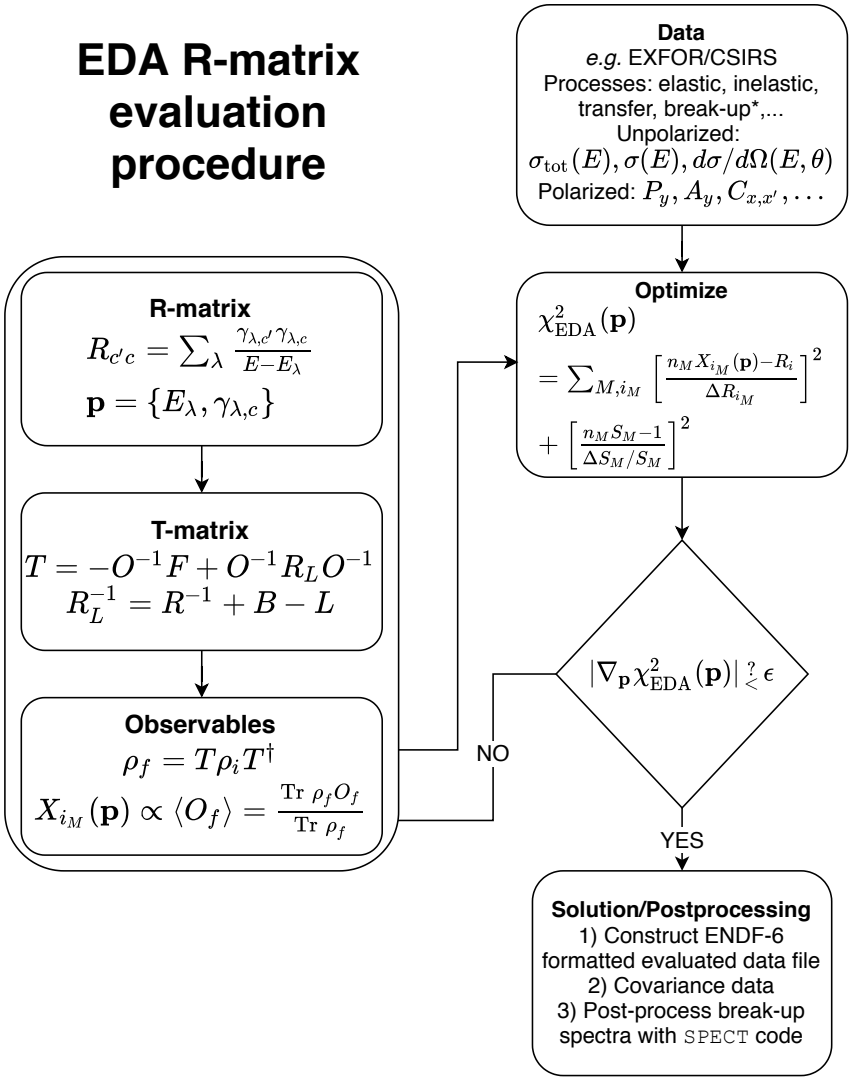
$$\Delta\chi^2_{\max} \approx k = \left\langle \Delta\chi^2 \right\rangle.$$

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

R-matrix evaluation

^{5}Li system

EDA R-matrix evaluation procedure



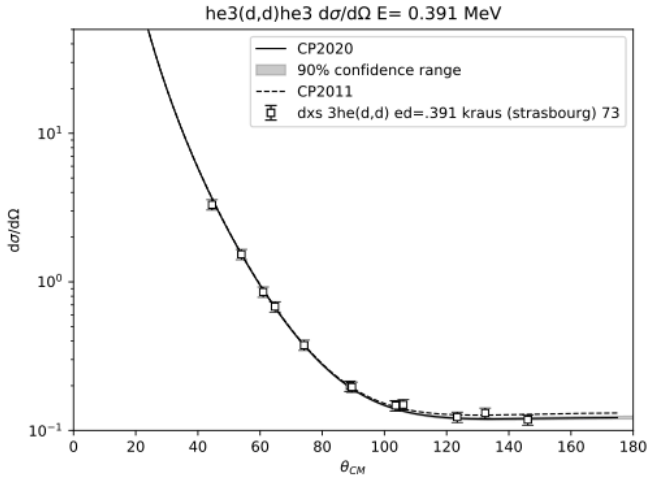
Channel	a_c (fm)	l_{max}
$d + ^3\mathrm{He}(\frac{1}{2}^+)$	4.8	4
$p + ^4\mathrm{He}(0^+)$	2.9	4
$p + ^4\mathrm{He}^*(0^+;\ 20.2\ \mathrm{MeV})$	3.4	2
$d_0 + ^3\mathrm{He}(\frac{1}{2}^+)$	5.1	0

Reaction	Energy Range (MeV)	# Data Points	Observables
$^3\mathrm{He}(d,d)^3\mathrm{He}$	$E_d = 0.32 - 10.0$	2,229	$\sigma(\theta), A_i, A_{ii}, C_{i,j}, C_{ij,k}, K_{i,j'k'}, K_{ij,k'l'}$
$^3\mathrm{He}(d,p)^4\mathrm{He}$	$E_d = 0.13 - 10.0$	3,839	$\sigma(E), \sigma(\theta), A_i, A_{ii}, C_{i,j}, K_{ij,k'}$
$^3\mathrm{He}(d,p)^4\mathrm{He}^*$	$E_d = 3.70 - 6.70$	28	$\sigma(\theta)$
$^4\mathrm{He}(p,p)^4\mathrm{He}$	$E_p = 0.92 - 34.3$	867	$\sigma(E), \sigma(\theta), A_y, P_y$
	Total:	6963	

Table 1: Channel configuration (top) and data summary (bottom) for the ^{5}Li system analysis. The column labeled "Observables" indicates the following data types: $\sigma(E)$, integrated cross section; $\sigma(\theta)$, unpolarized angular distributions (energy-dependence suppressed); A initial-state analyzing power; P final-state polarization; C spin correlation coefficients; K polarization transfer coefficients. (We have suppressed the indices $i, j, \ldots$ which take on values x, y, z for spins/polarization directions in configuration space.) All polarization and spin distributions are angular distributions, which depend on the angle of the outgoing particle. Chi-squared per degree of freedom for the analysis is $\chi^2/\mathrm{dof} \simeq 2.7$ over 7,178 data points, 215 of which were discarded by eliminating individual data points which contribute to $\chi^2 > 40$.

^{5}Li system evaluation

^{3}He(d,d)^{3}He



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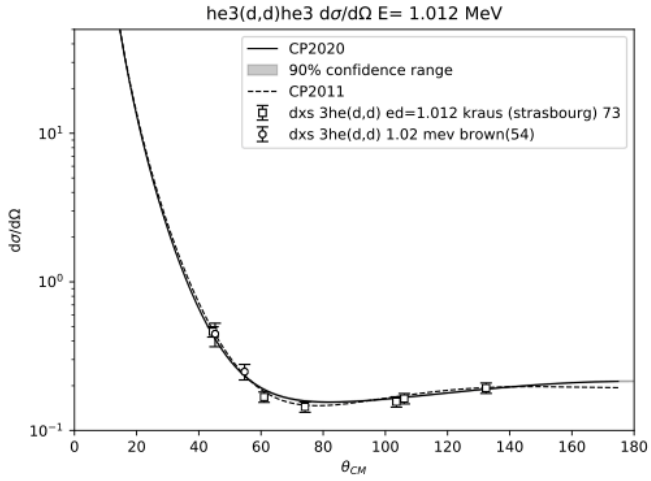

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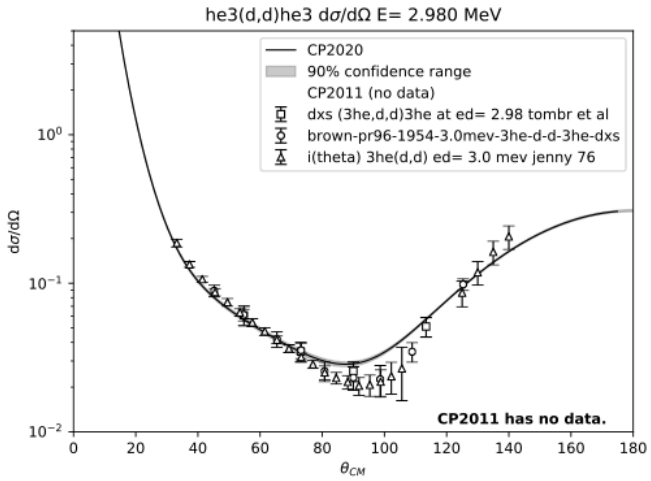

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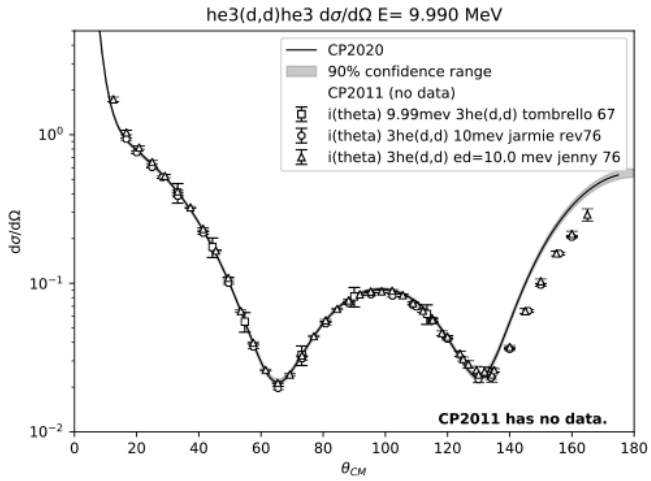
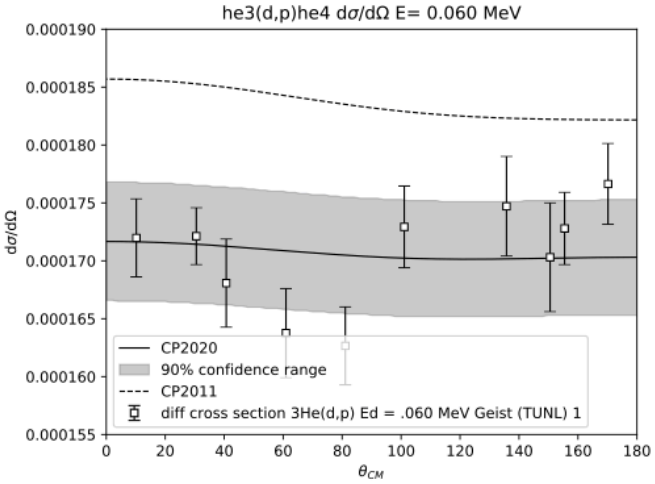


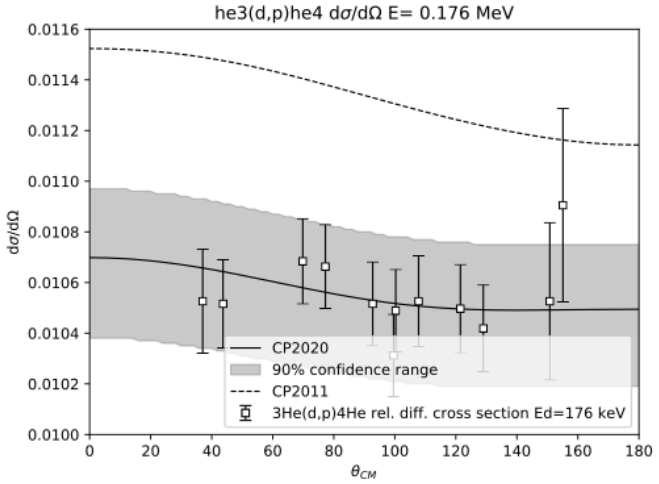
(d)

^{5}Li system evaluation

^{3}He(d,p)^{4}He



(a)



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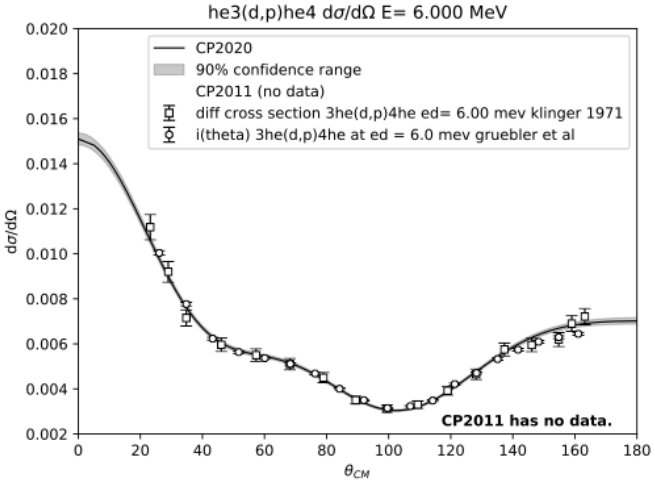

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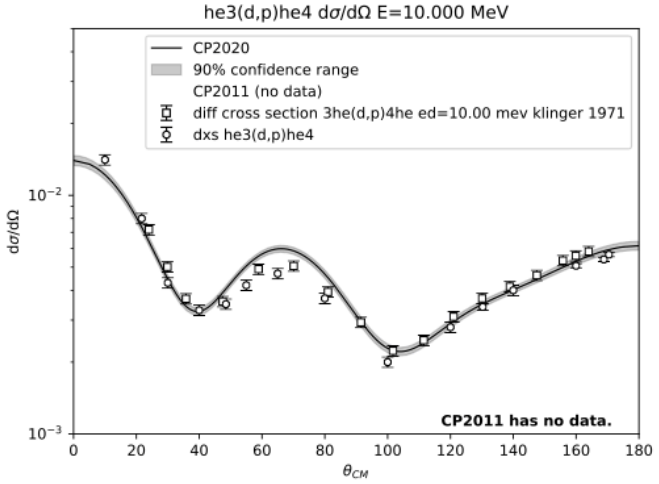
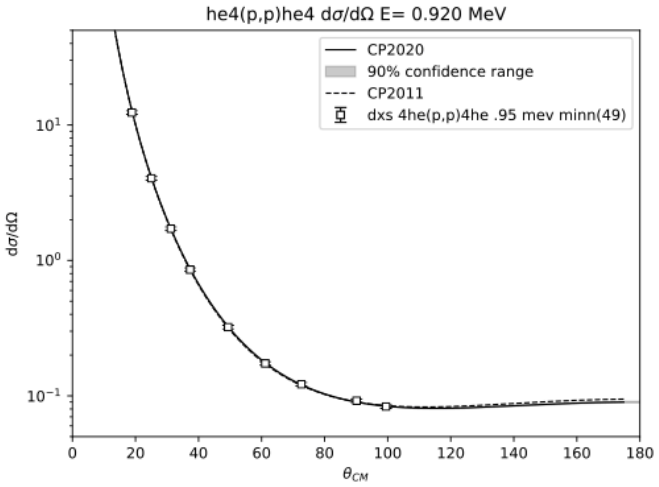


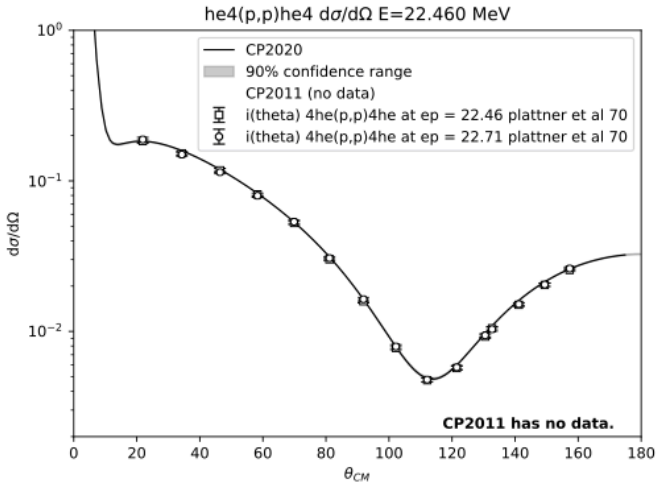
(d)

^{5}Li system evaluation

^{4}He(p,p)^{4}He



(a)



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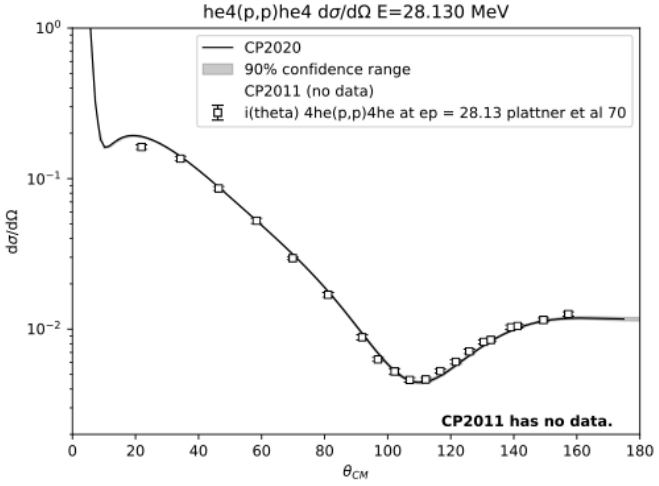

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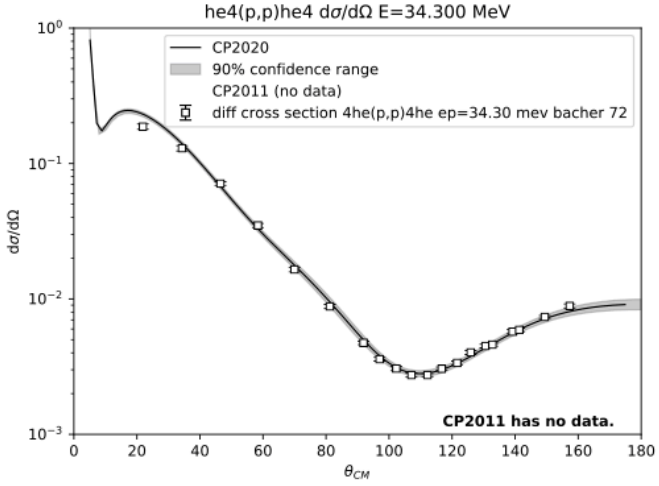


(d)

NN evaluation: configuration & data

- Neutron energies $E_n \leqq 50$ MeV
- Charge-independent analysis

$$R(E) = \sum_{\lambda,T} \frac{\gamma_\lambda^{(T)} \tilde{\gamma}_\lambda^{(T)}}{E_\lambda^{(T)} - E}.$$

  - T=1 (pp, np-isovector)
  - T=0 (np-isoscalar)
  - Coulomb energy-level shift

$$E_\lambda^{(T=1)} = E^{(T=0)} + \Delta_Z$$

    - Fit to $a_{nn} = -18.5$ fm
  - Predict nn scattering
- High-fidelity description

$$\chi^2/\mathrm{dof} = 0.9$$

- Planned evaluation
  - $E_n \lesssim 250$ MeV

TABLE II. Channel configuration (top) and data summary (bottom) for the charge-independent $N-N$ analysis up to 50 MeV. Since the number of free parameters is 43 resonance parameters + 83 normalizations, the chi-squared per degree of freedom for the analysis is 0.90.

Channel	a_c (fm)	$l_{\max}$
$p+p$	3.26	3
$n+p$	3.26	3
$\gamma+d$	84.6	1
$n+n$	3.26	3

Reaction	# Pts.	χ^2	Observable Types
$p(p,p)p$	675	951	$\sigma(\theta), A_y(p), C_{x,x'}, C_{y,y'}, K_x^{x'}, K_y^{y'}, K_z^{x'}$
$p(n,n)p$	4815	3764	$\sigma_{\mathrm{T}}, \sigma(\theta), A_y(n), C_{y,y'}, K_y^{y'}$
$p(n,\gamma)d$	86	179	$\sigma_{\mathrm{int}}, \sigma(\theta), A_y(n)$
$d(\gamma,n)p$	88	77	$\sigma_{\mathrm{int}}, \sigma(\theta), \Sigma(\gamma), P_y(n)$
$n(n,n)n$	1	0	a_0
Norms.	80	86	
Total:	5745	5057	20

Integrated cross sections

Comparison with ENDF/B-VIII.0

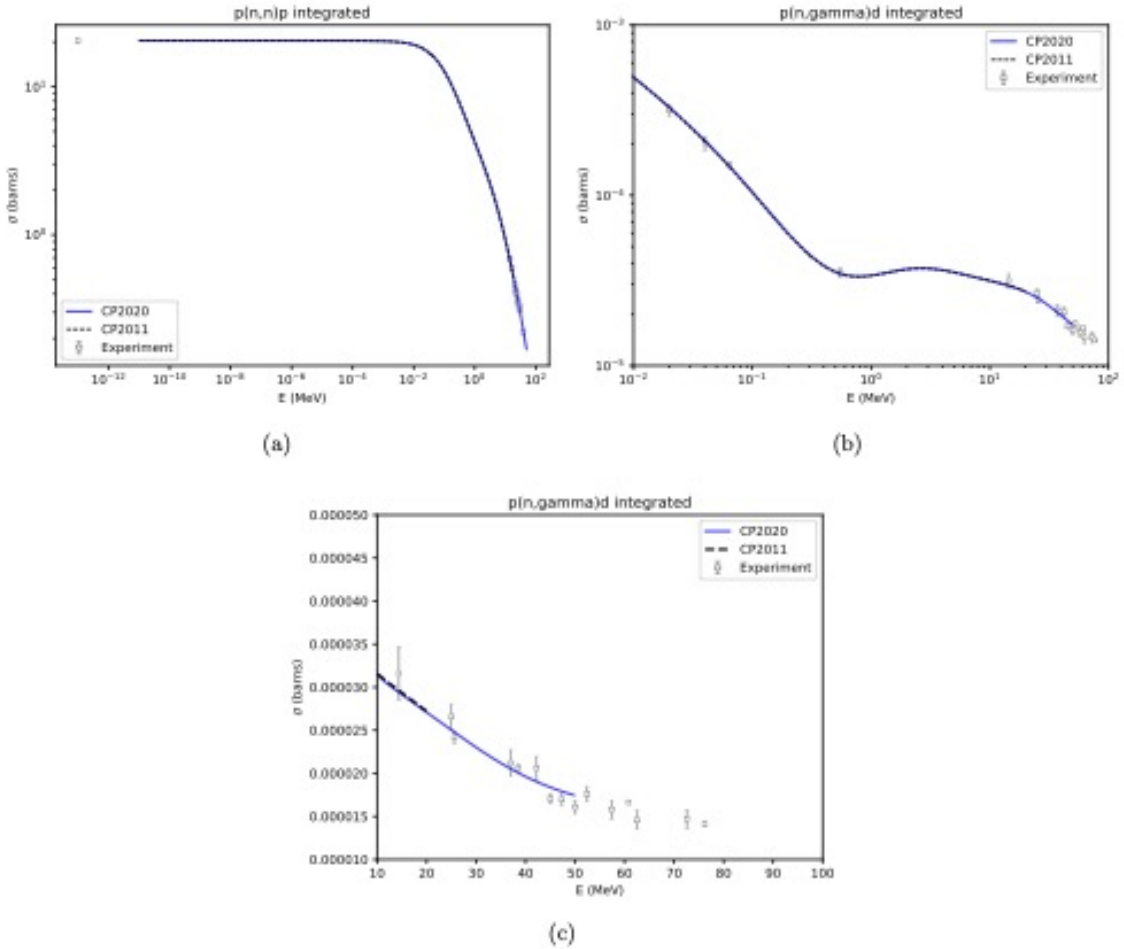
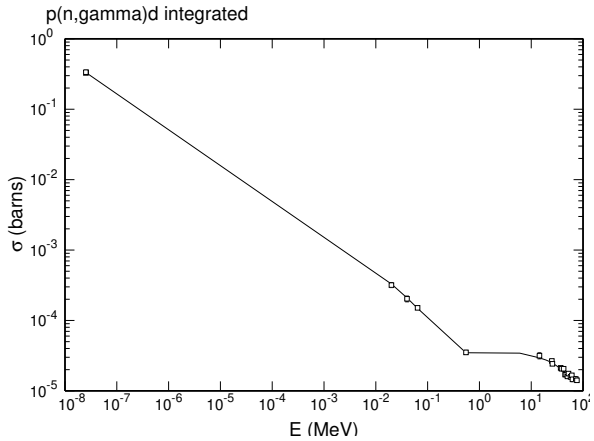
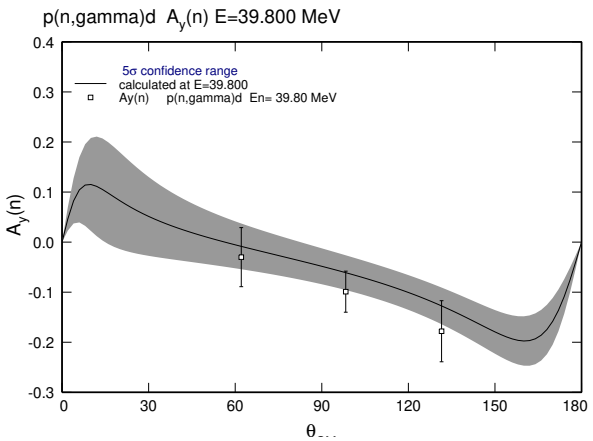
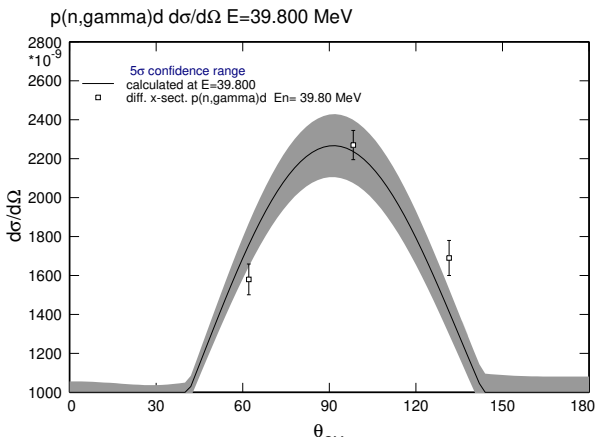


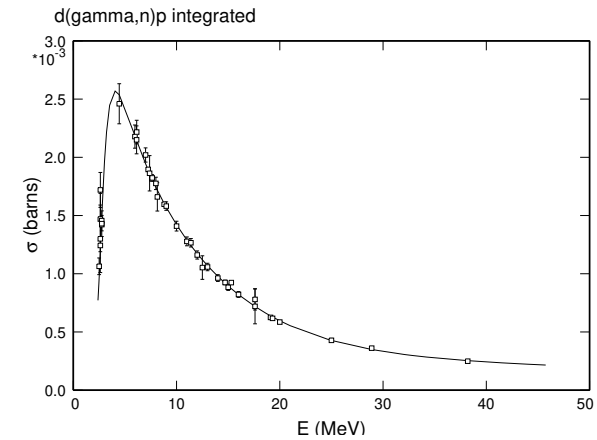
Figure 6: The CP2020 integrated cross sections (solid, blue curves) compared with those of CP2011 (dashed curves) and the experimentally observed data for: (a) $^1\mathrm{H}(n,n)^1\mathrm{H}$ reaction; (b) $^1\mathrm{H}(n,\gamma)^2\mathrm{H}$ reaction; (c) $^1\mathrm{H}(n,\gamma)^2\mathrm{H}$ reaction (focus on high-energy region). The capture process $^1\mathrm{H}(n,\gamma)^2\mathrm{H}$ has not yet been updated in an ENDF file for CP2020.

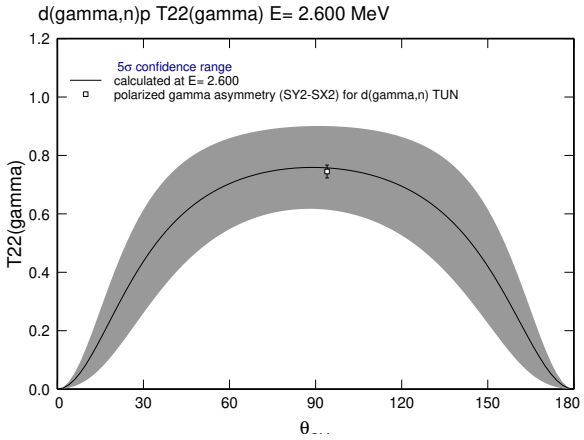
n+p Capture and γ+d Photodisintegration Data

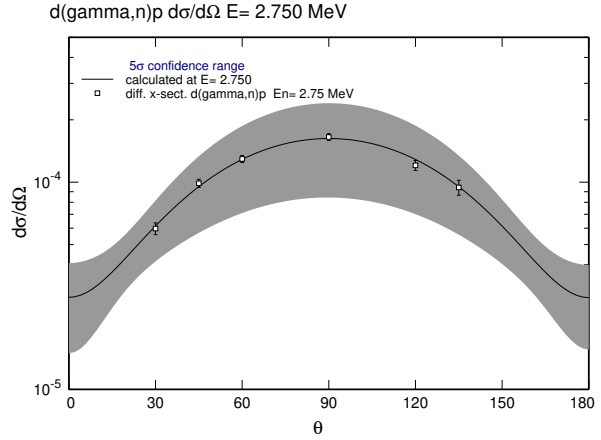




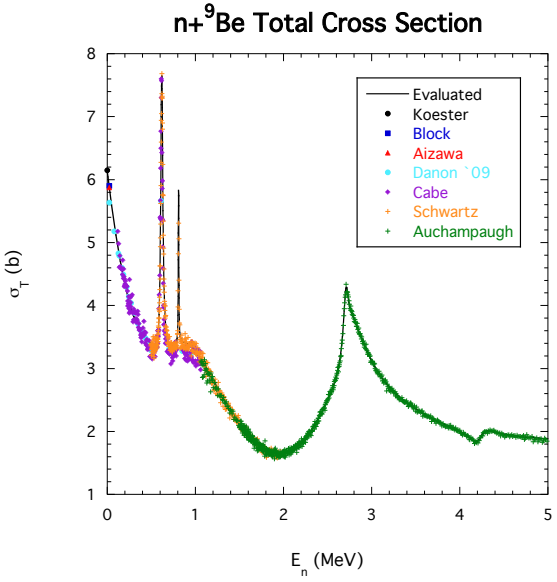


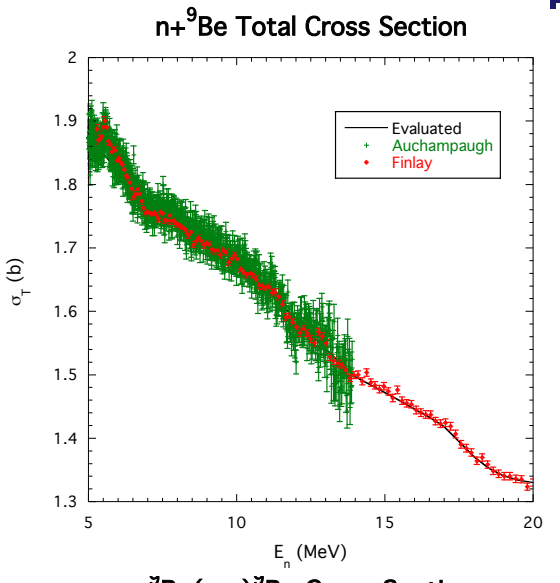


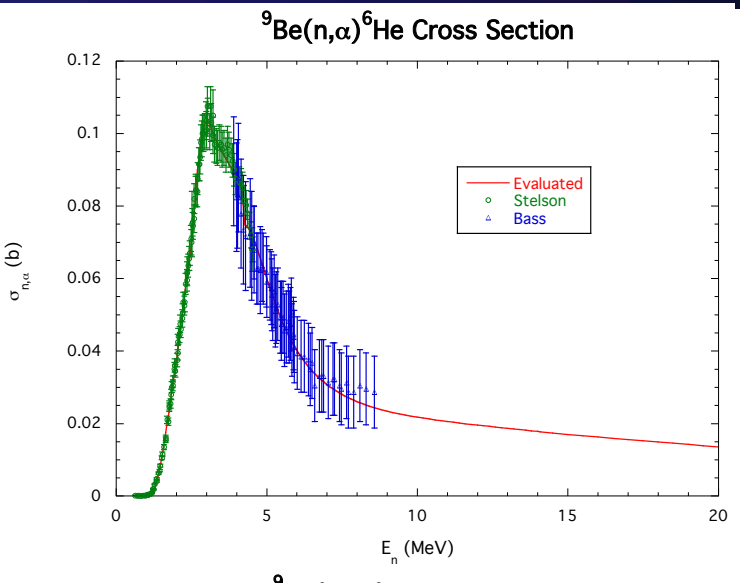


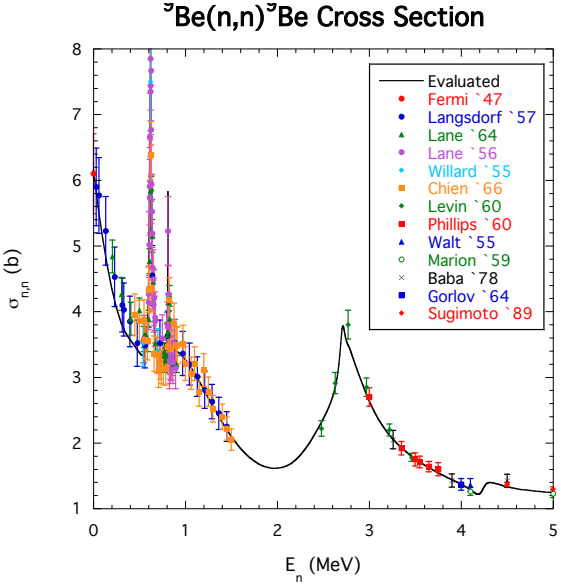


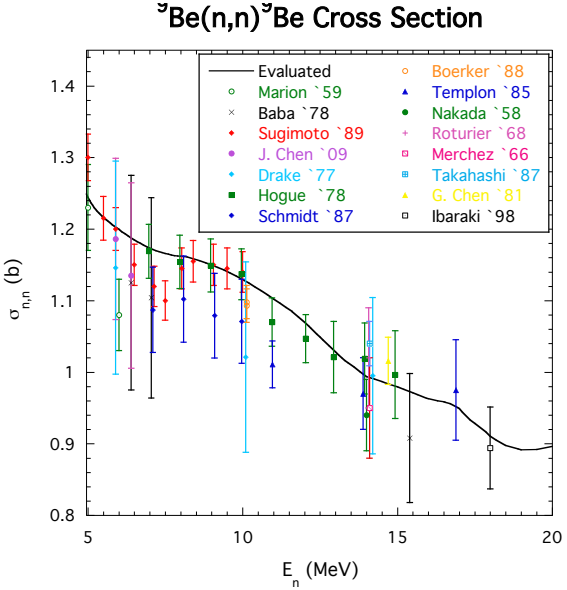
n+^{9}Be Integrated Cross Sections

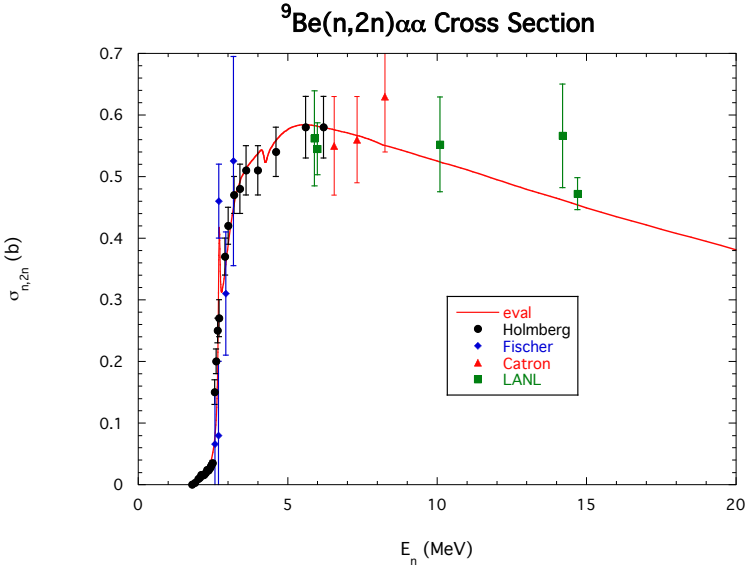




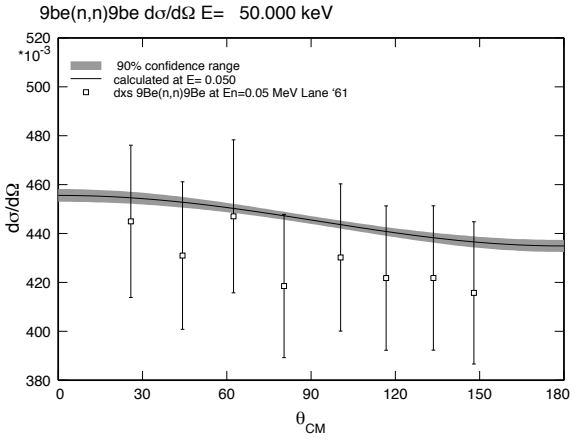


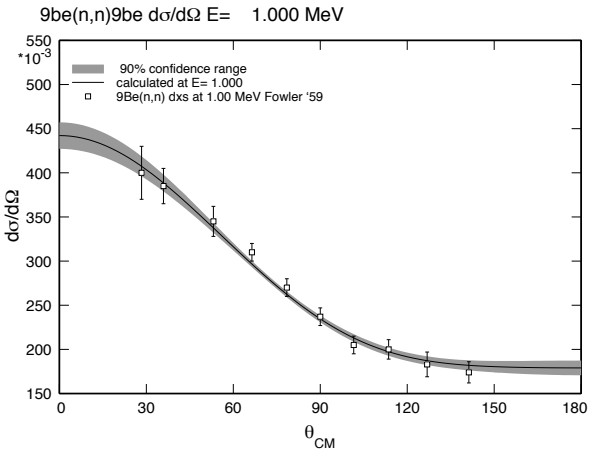


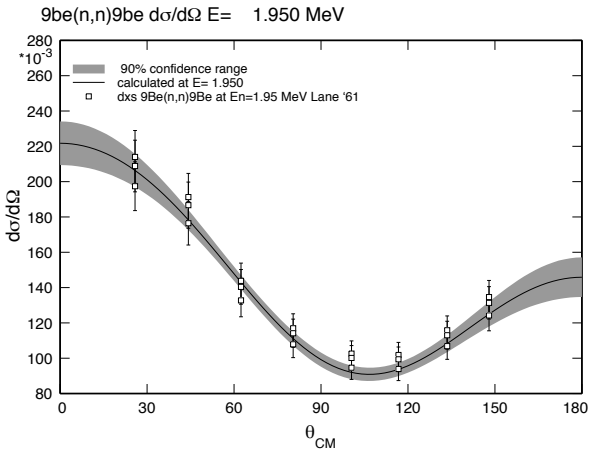


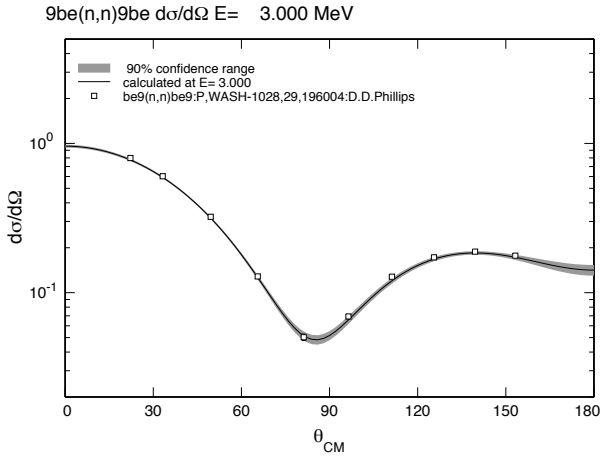


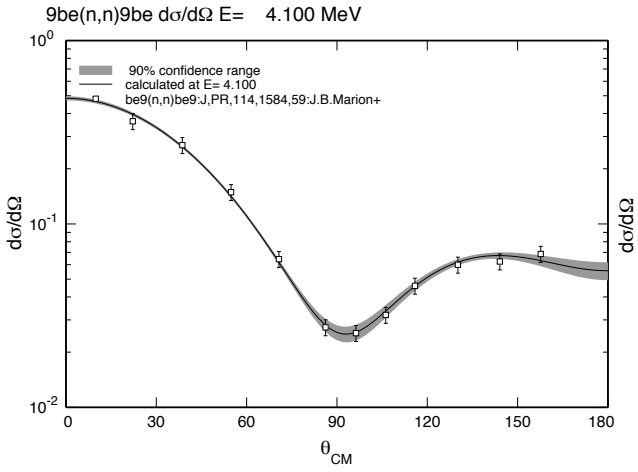
^{9}Be(n,n)^{9}Be Differential Cross Sections

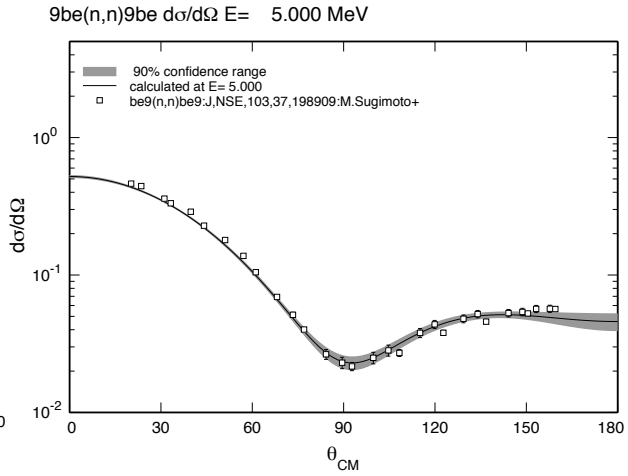




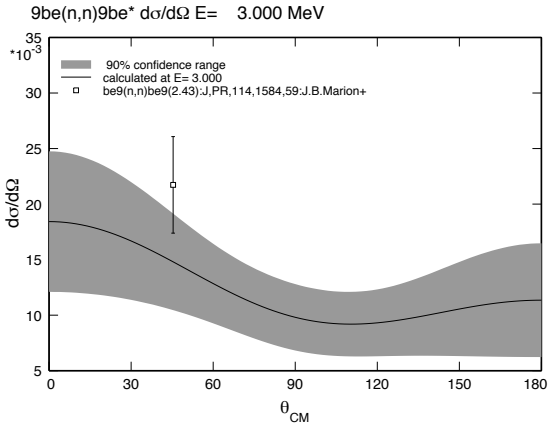


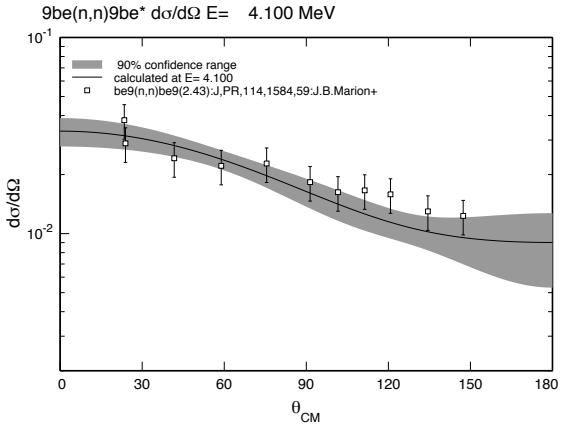


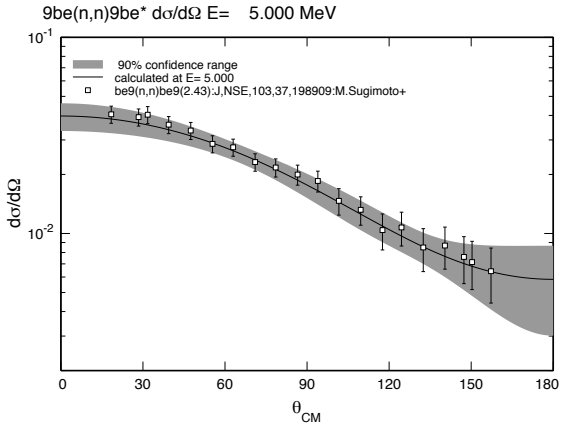




$^{9}Be(n,n_2)^{9}Be^{**}$ Differential Cross Sections







SUMMARY:

- ^{10}Be analysis has produced a consistent set of cross sections and angular distributions that are in agreement with most of the experimental data at energies up to 5 MeV. Extensions above that energy were based on the experimental data alone.
- Level assignments for the overlapping resonances near E_n=2.7 MeV have the opposite parity ($4^-,3^+ \rightarrow 4^+,3^-$).
- Excited states of ^{9}Be make important contributions to the (n,2n) cross section (MT=16 → 24 in the new evaluation).
- We are making comparisons of the new evaluation to integral benchmarks (M. Herman, LANL) and thick-target angular neutron yields (Y. Danon, RPI).


Thank you.