# Evaluation updates for $^{9}$Be and charged particles

CSEWG
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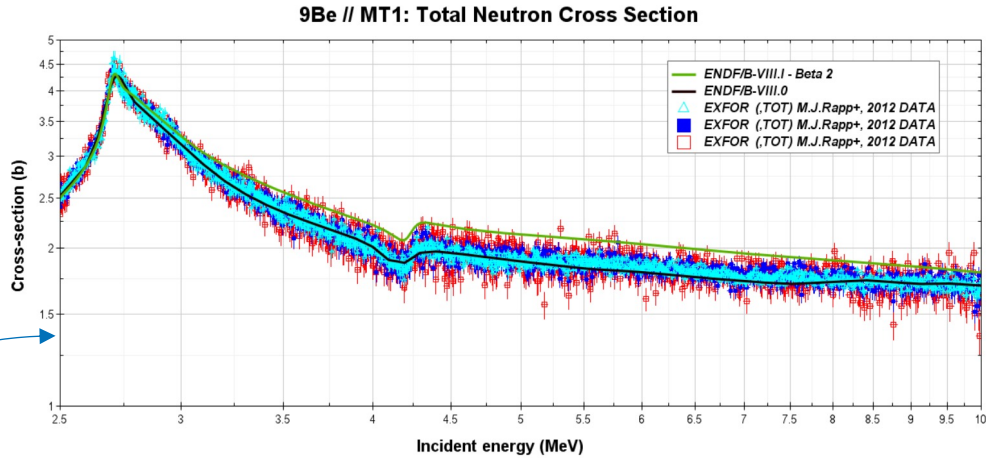
# Outline

- Evaluation updates for ENDF/B-VIII.1β2
  - n+$^{9}$Be
  - Charged particle sublibraries

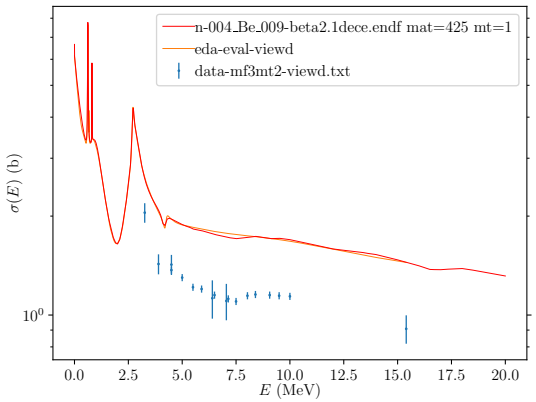
# $^{9}Be$

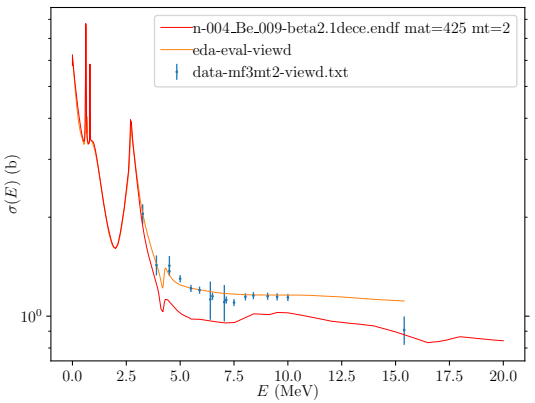
# n+$^{9}$Be evaluation summary

- Reminder of R-matrix evaluation
  - Increased elastic angular distros
  - Introduced new channels
    - (n,n$_1$) & (n,$\gamma$)
  - Upper energies in R-matrix evaluation increased

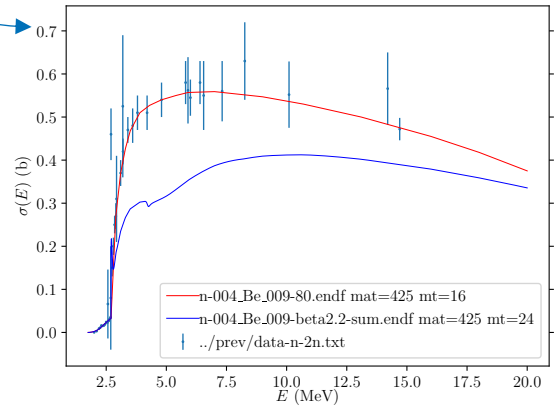



- Yaron pointed out MT1 issue
  - Revealed inconsistency between
    - MT24 (n,2nα)+MT52(n,n$_1$)
    - MT1 & MT2




- Possible solutions
  - Reduce MT24 by MT52
    - **Rejected**: requires LR≠ 0
  - Remove MT52 information
    - **Favored**
    - Postpone resolution to ENDF/B-IX



# n+$^{9}$Be

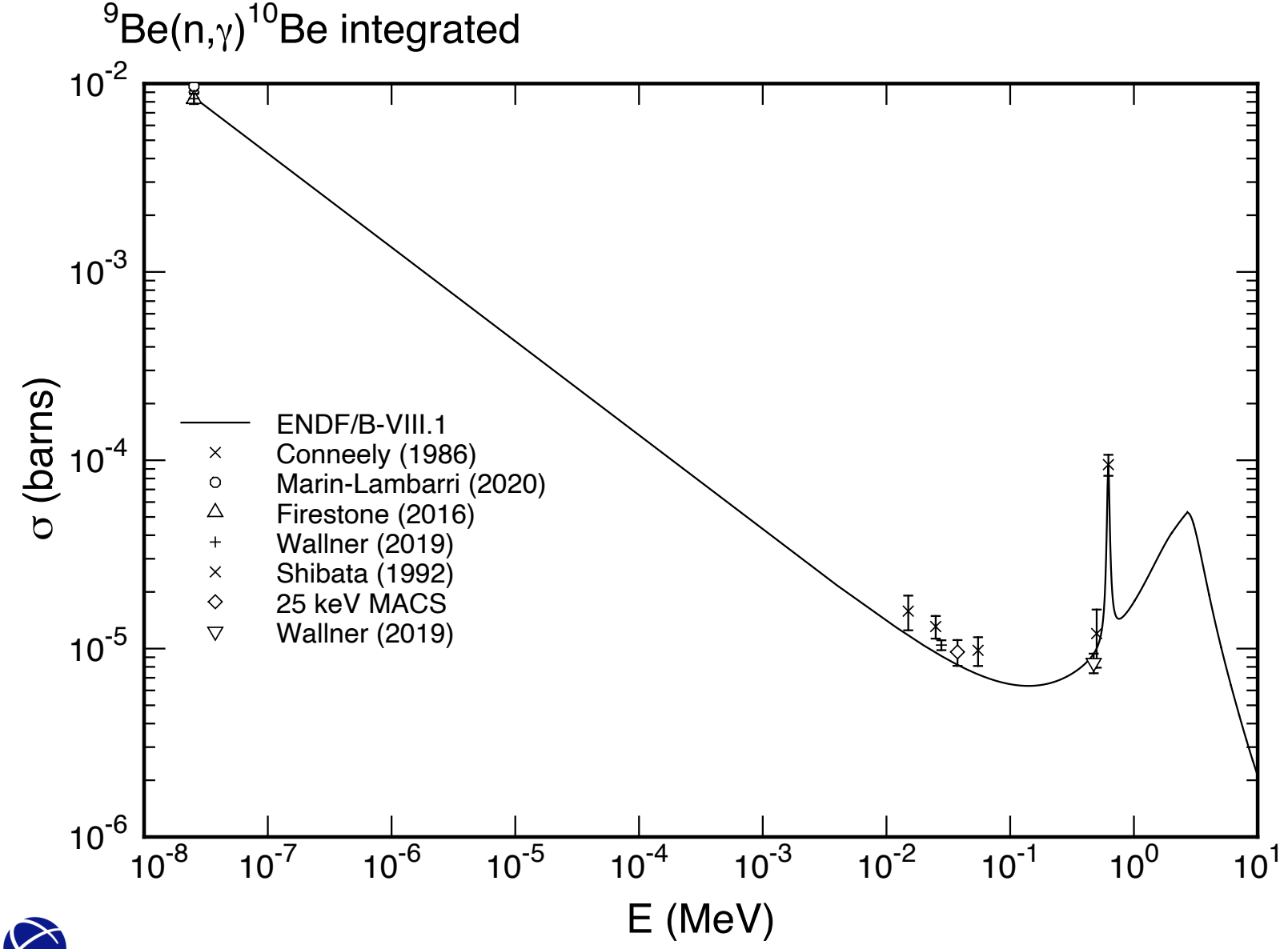
## *R-matrix configuration*

| Channel | $a_c$(fm) | $\ell_{\max}$ |
|---|---|---|
| $n$+$^{9}$Be($\frac{3}{2}^-$) | 4.67 | 3 |
| $^{4}$He +$^{6}$He($0^+$) | 5.00 | 4 |
| $(nn)_0$+$^{8}$Be($2^+$) | 5.20 | 3 |
| $n$ +$^{9}$Be*($\frac{5}{2}^-$) | 5.20 | 1 |
| $\gamma$ +$^{10}$Be | 50.0 | 3 |

| Process | $E_n$ range | Observables | $N_{\rm dat}$ | $\chi^2/N_{\rm dat}$ |
|---|---|---|---|---|
| $^{9}$Be$(n,n_0)^{9}$Be | (1.25 eV, 15.4 MeV) | $\sigma_{\rm tot}, \sigma, \sigma(\theta), A_y(\theta)$ | 5782 | 1.65 |
| $^{9}$Be$(n,^{4}$He$)^{6}$He | (0.63, 8.5) MeV | $\sigma, \sigma(\theta)$ | 178 | 1.40 |
| $^{9}$Be$(n,2n)^{8}$Be | (1.8, 14.7) MeV | $\sigma$ | 40 | 13.95 |
| $^{9}$Be$(n,n_1)^{9}$Be* | (2.7, 5.0) MeV | $\sigma(\theta)$ | 83 | 1.65 |
| $^{9}$Be$(n,\gamma)^{10}$Be | (.0253 eV, .6 keV) | $\sigma$ | 11 | 1.90 |
| Total | | | 6094 | 1.75 |

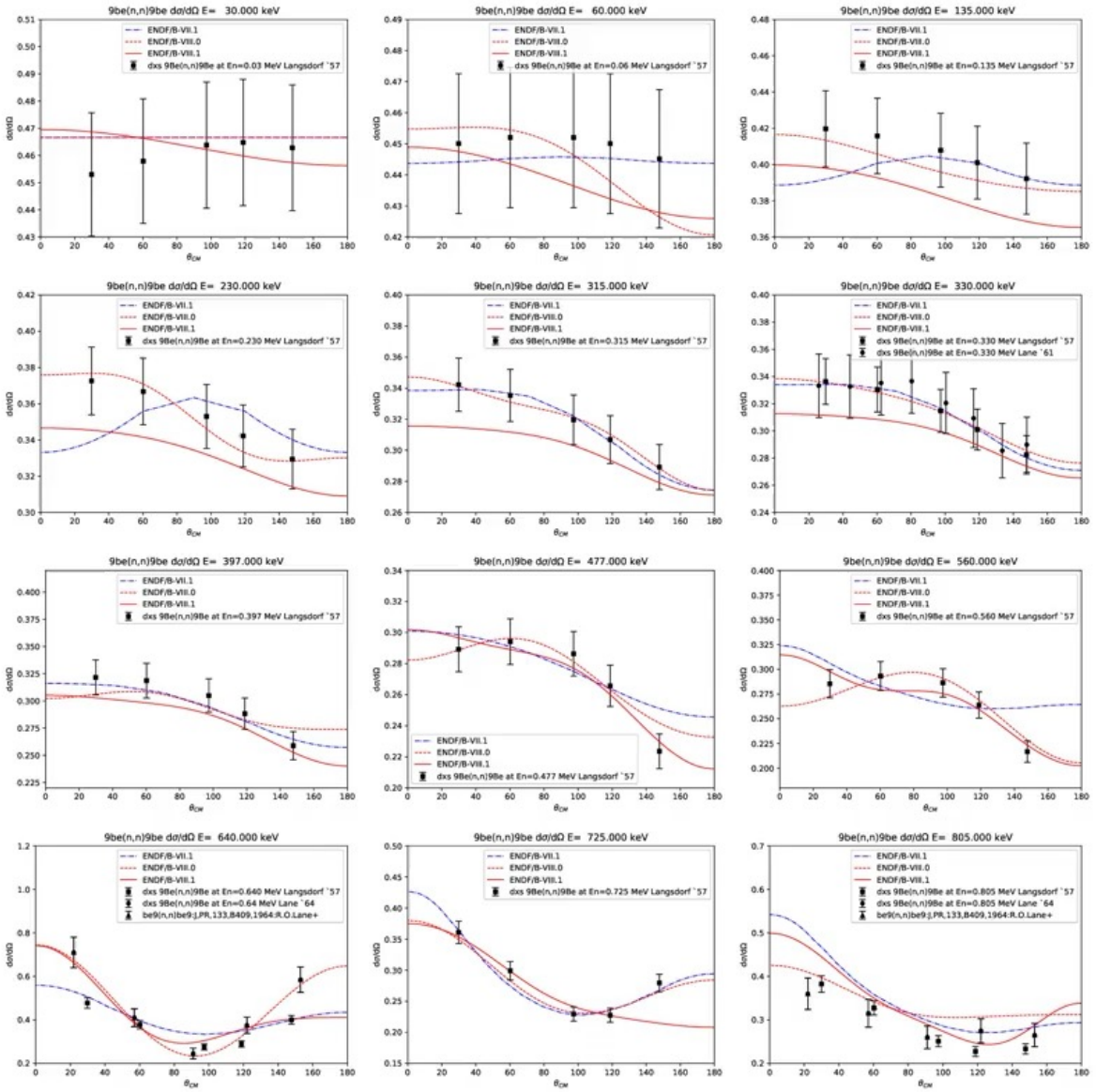
- Added data: elastic, (n,$\alpha$), (n,n$_1$), (n,$\gamma$)
- Upper energy
  - $E_n$ < 15.4 MeV (total and integrated cross sections)
  - Extended from 1.6 MeV to 5.0 MeV (elastic and inelastic angular distributions)

# Capture


$^{9}Be(n,\gamma)^{10}Be$ integrated
σ (barns)
E (MeV)
ENDF/B-VIII.1
Conneely (1986)
Marin-Lambarri (2020)
Firestone (2016)
Wallner (2019)
Shibata (1992)
25 keV MACS
Wallner (2019)

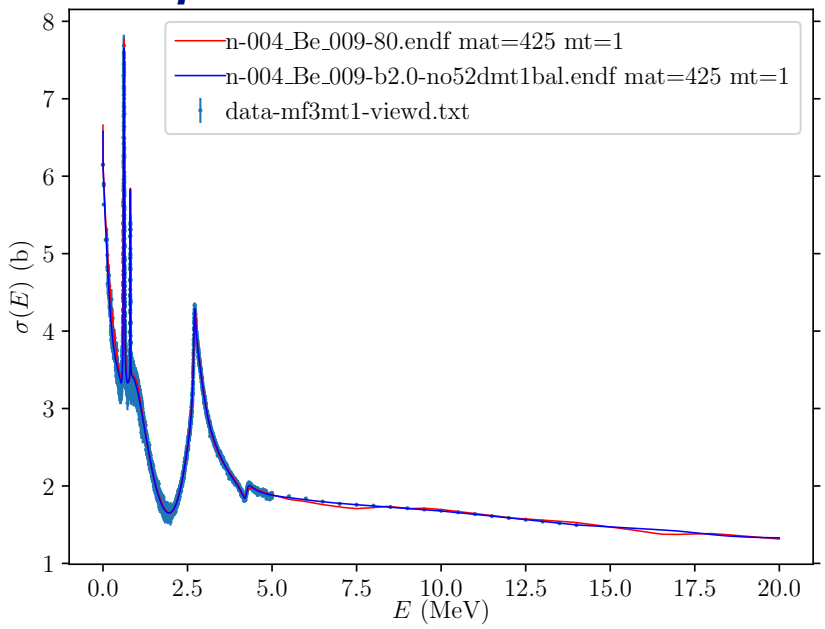
# Angular distributions

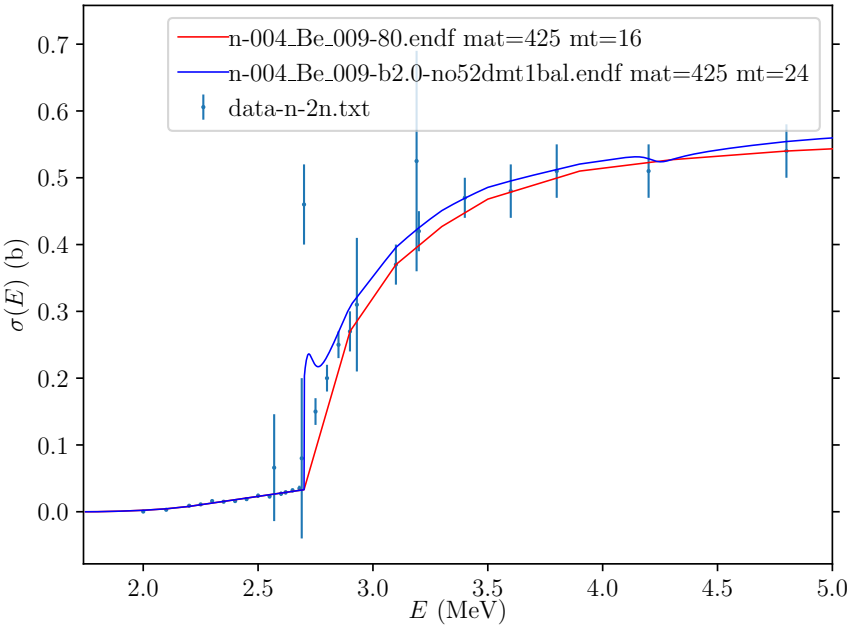
- Fit quality ranges from is relatively high (n,el) to “OK” (n,n’)
- Comparison
  - ENDF/B-VII.1
  - ENDF/B-VIII.0
  - ENDF/B-VIII.1β2.1
- Processes
  - Elastic
  - (n,a)
  - (n,n1)

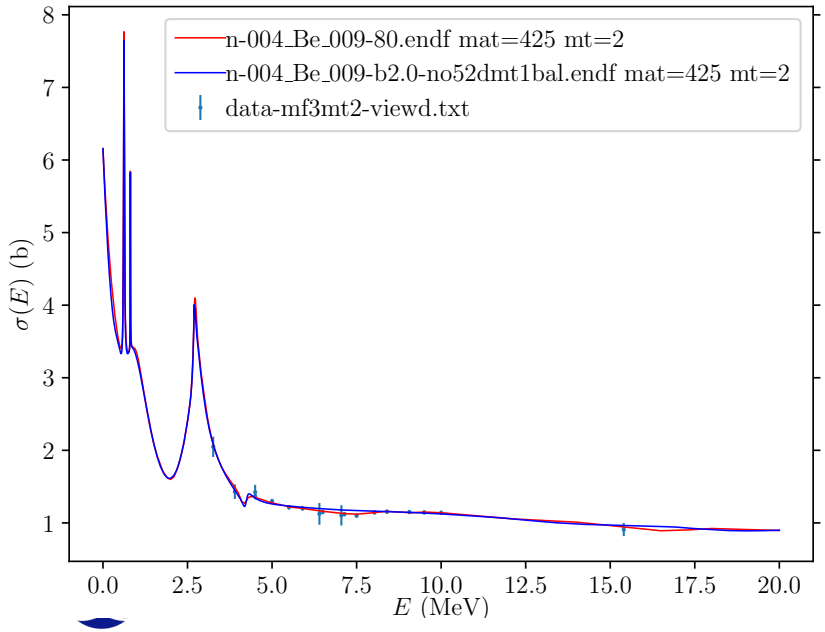


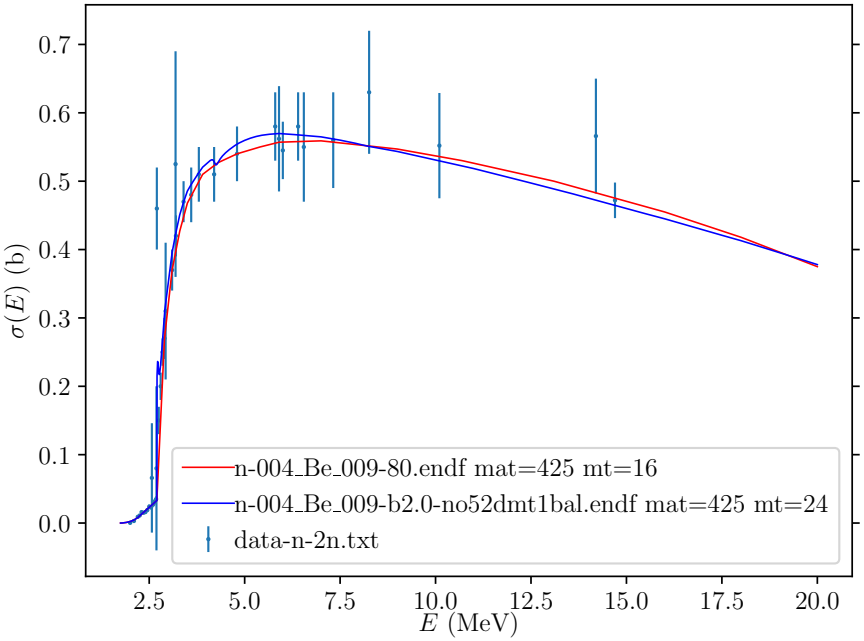
# $^{9}$Be(n,2n)

## *VIII.1β2.1*



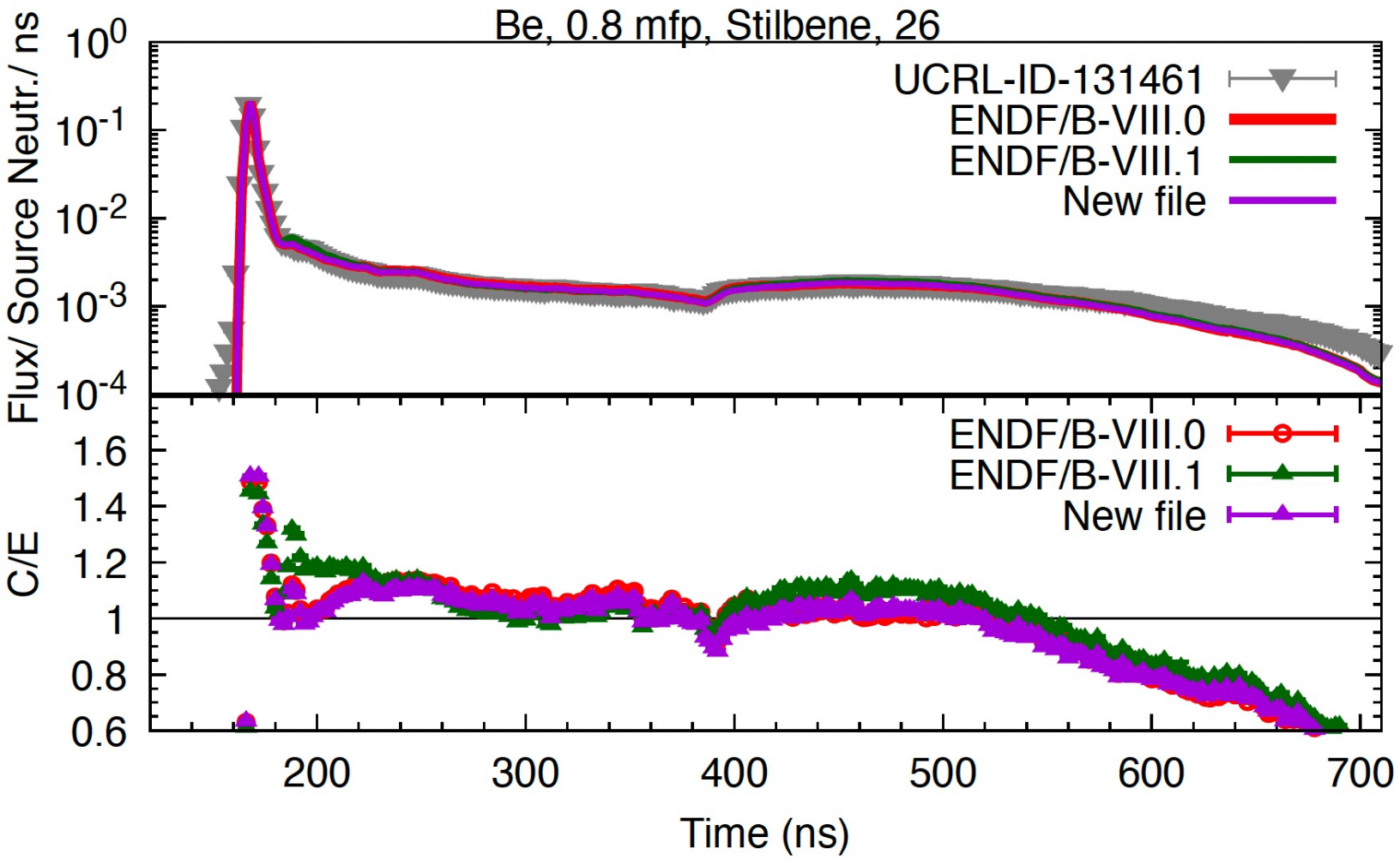



# n+$^{9}$Be integral testing

## *LLNL Pulsed spheres—Neudecker (LANL)*




- Removing MT52 addresses Be pulsed sphere problem at high energy

# Be in Various HMFs and PMFs

## Skip Kahler

Now showing E80, e81β1 plus the first and third attempts to fix $^{9}$Be.

E80 splits the E70, E71 difference …

- $k_{ave}$(E80) = 0.99938 ± 0.00273

E81β1 was also good, but e81β2+fix9Be and fix9Be3 remain below the too cool E70

- $k_{ave}$(E70) = 0.99815 ± 0.00371
- $k_{ave}$(e81β1) = 0.99978 ± 0.00347
- $k_{ave}$(e81β2+fix9Be) = 0.99695 ± 0.00336
- $k_{ave}$(e81β2+fix9Be3) = 0.99710 ± 0.00356

BeRP Ball, PMF38, is best with E80

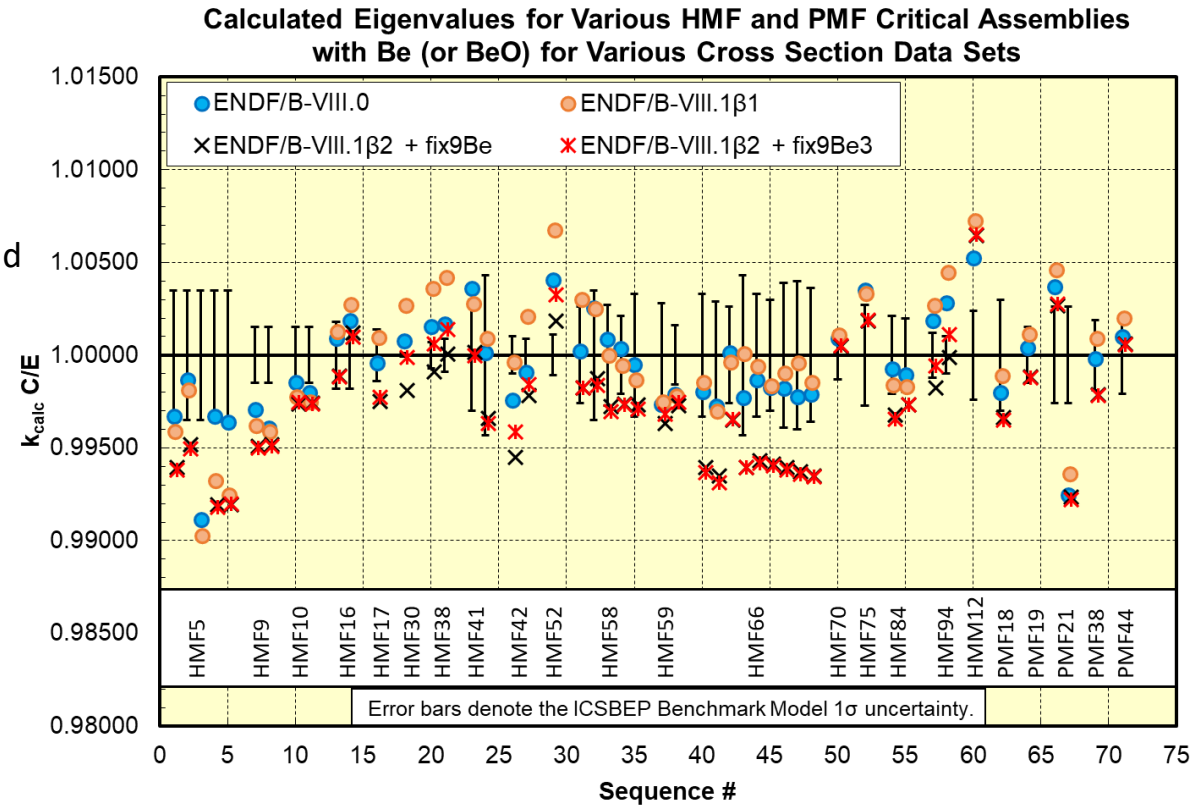
($k_{calc}$C/E = 0.99981(4))

but drops to

0.99788(7) with e81β2+fix9Be

and

0.99783(7) with e81β2+fix9Be3.

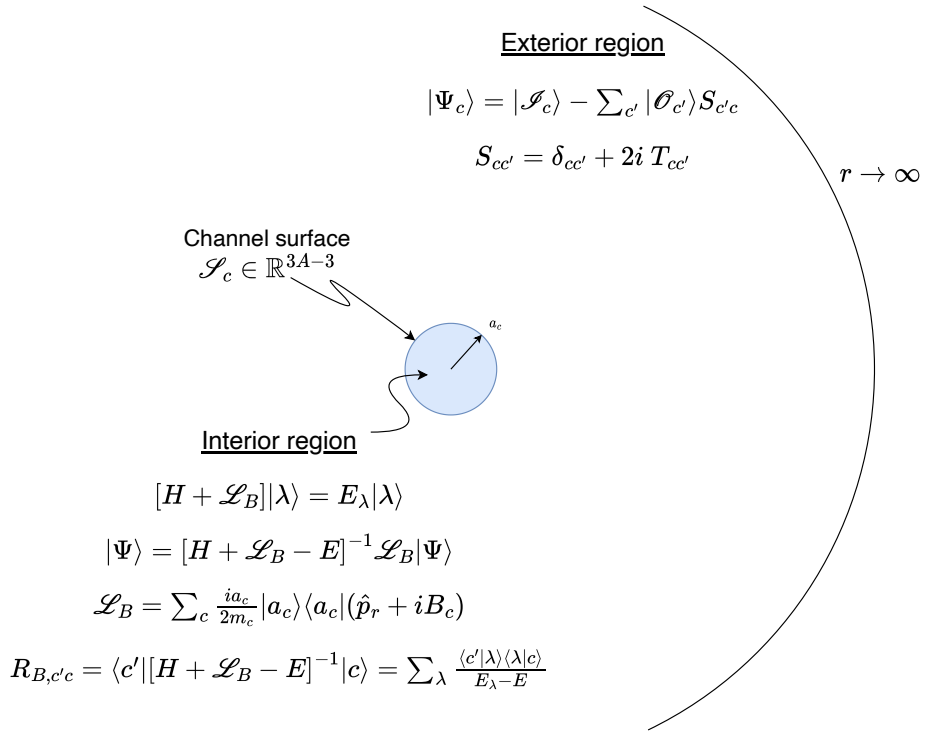


# Charged-particle sublibraries

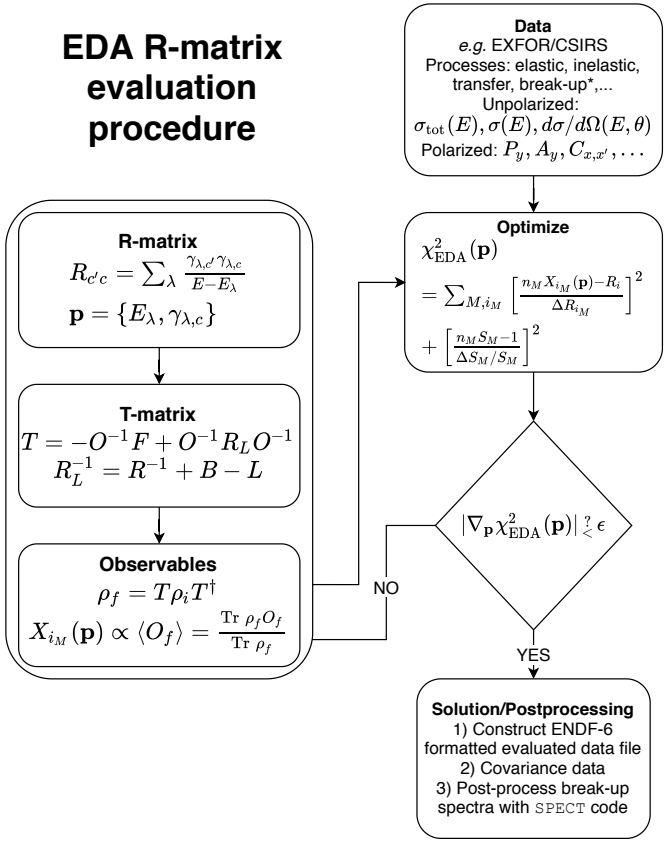
# Outline

- R-matrix formalism
- Charged particle sublibrary
  - $^{5}$Li system
- MF2 resonance parameters
  - $^{5}$He test
- **What is the history of the current d-001_H_003.endf file?**

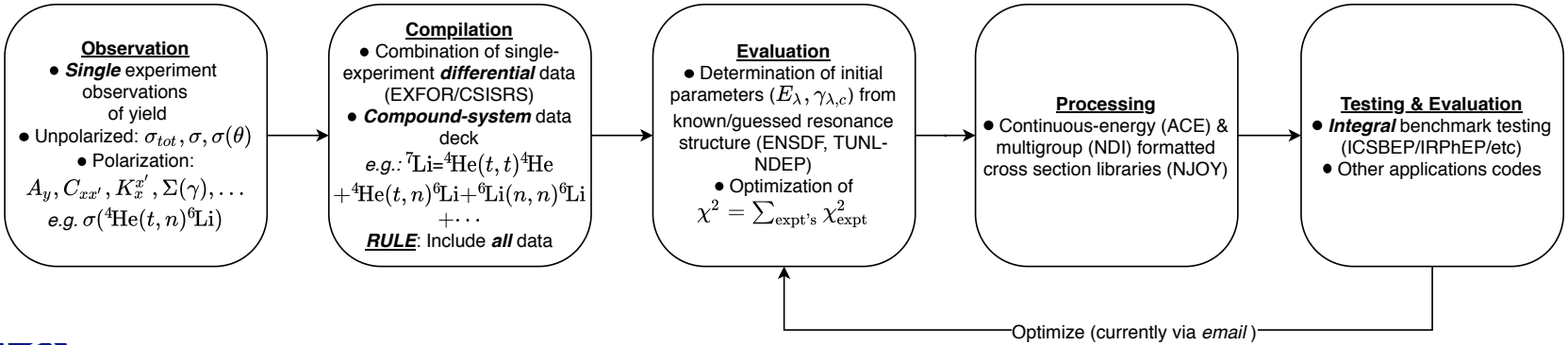
# R-matrix formalism




## EDA R-matrix evaluation procedure




## Nuclear Data Pipeline
### *EDA* cross section evaluation



# LANL light-element program

- All compound systems A<20 (and a few above)
- Recent work in 2020:

| 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 |
| $h(^{3}\mathrm{He})$ | | | | VIII.0 | VIII.0 | VIII.0 | TENDL09 |
| $\alpha$ | | | | | VIII.0 | TENDL09 | TENDL09 |

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

# Overview

## *Proposed additions/revisions to ENDF/B library*

- **Tapes – all extended energy/better agreement with more data; Covariances planned**
  - `p-002_He_004.endf [ready] -> [submitted-phase1]`
  - `d-002_H_003.endf [checking]`
  - `d-002_He_003.endf [submitted]`
  - `d-003_Li_006.endf [ready]`
  - `n-003_Li_006.endf [submitted]`
  - `t-002_He_004.endf [ready] -> [submitted-phase1]`

- **Testing**
  - NJOY
  - IAEA/Dunford codes [checkr, stanef, fizcon, psyche, inter]
  - ENDF > ACE
    - checkace [LANL ACE format checking tool]
    - mcnp6.1 pencil beam (d+3He only)
- **Comparisons**
  - with ENDF/B-VII.1 (*aka*, "CP2011"), VIII.0
  - with LLNL *Evaluated Charged Particle Library (ECPL-2018)*

# Changes

## d-002_He_003.endf

| MF | MT | Description | Energy range [MeV] |
|---|---|---|---|
| 3 | | Reaction cross sections | |
| | 2 | (z,z0) | ( 0.01, 1.40) |
| | 600 | (z,$p_0$) | ( 0.00, 1.40) |
| 6 | | Energy-angle distributions for emitted particles | |
| | 2 | (z,z0) | |
| | 600 | (z,$p_0$) | |

Table 26: ENDF/B-VIII.0 library, file: d-002_He_003.endf

| MF | MT | Description | Energy range [MeV] |
|---|---|---|---|
| 3 | | Reaction cross sections | |
| | 2 | (z,z0) | ( 0.01, 20.00) |
| | 600 | (z,$p_0$) | ( 0.01, 20.00) |
| 6 | | Energy-angle distributions for emitted particles | |
| | 2 | (z,z0) | |
| | 600 | (z,$p_0$) | |

Table 27: CP2020 library new evaluation, file: d-002_He_003.endf

# Changes

## p-002_He_004.endf

| MF | MT | Description | Energy range [MeV] |
|---|---|---|---|
| 3 | | Reaction cross sections | |
| | 2 | (z,z0) | ( 0.11, 20.00) |
| 6 | | Energy-angle distributions for emitted particles | |
| | 2 | (z,z0) | |

Table 86: ENDF/B-VIII.0 library, file: p-002_He_004.endf

| MF | MT | Description | Energy range [MeV] |
|---|---|---|---|
| 3 | | Reaction cross sections | |
| | 2 | (z,z0) | ( 0.02, 34.30) |
| | 650 | (z,$d_0$) | ( 23.02, 34.30) |
| 6 | | Energy-angle distributions for emitted particles | |
| | 2 | (z,z0) | |
| | 650 | (z,$d_0$) | |

Table 87: CP2020 library new evaluation, file: p-002_He_004.endf

# Changes

## t-002_He_004.endf

| MF | MT | Description | Energy range [MeV] |
|---|---|---|---|
| 3 | | Reaction cross sections | |
| | 2 | (z,z0) | ( 0.14, 20.00) |
| 6 | | Energy-angle distributions for emitted particles | |
| | 2 | (z,z0) | |

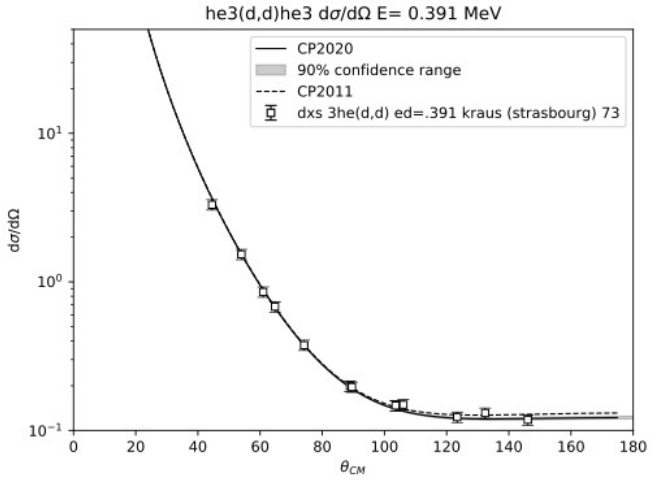
Table 120: ENDF/B-VIII.0 library, file: t-002_He_004.endf

| MF | MT | Description | Energy range [MeV] |
|---|---|---|---|
| 3 | | Reaction cross sections | |
| | 2 | (z,z0) | ( 0.10, 20.00) |
| | 50 | (z,$n_0$) | ( 8.39, 20.00) |
| | 51 | (z,$n_1$) | ( 12.28, 20.00) |
| | 52 | (z,$n_2$) | ( 14.65, 20.00) |
| | 600 | (z,$p_0$) | ( 13.18, 20.00) |
| | 650 | (z,$d_0$) | ( 10.98, 20.00) |
| 6 | | Energy-angle distributions for emitted particles | |
| | 2 | (z,z0) | |
| | 50 | (z,$n_0$) | |
| | 51 | (z,$n_1$) | |
| | 52 | (z,$n_2$) | |
| | 600 | (z,$p_0$) | |
| | 650 | (z,$d_0$) | |

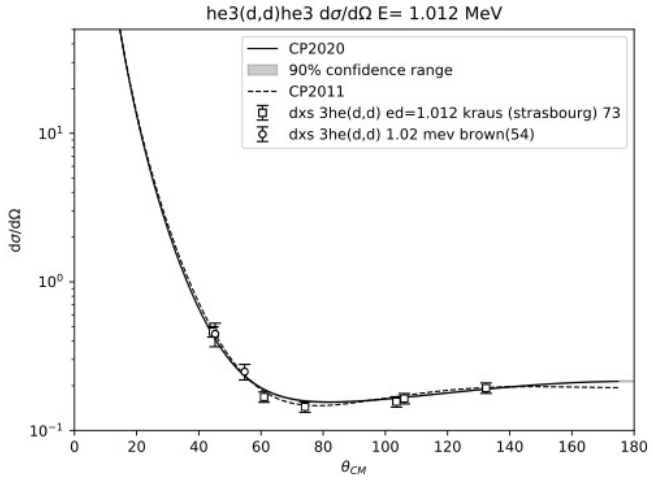
Table 121: CP2020 library new evaluation, file: t-002_He_004.endf

# $^{5}$Li system evaluation

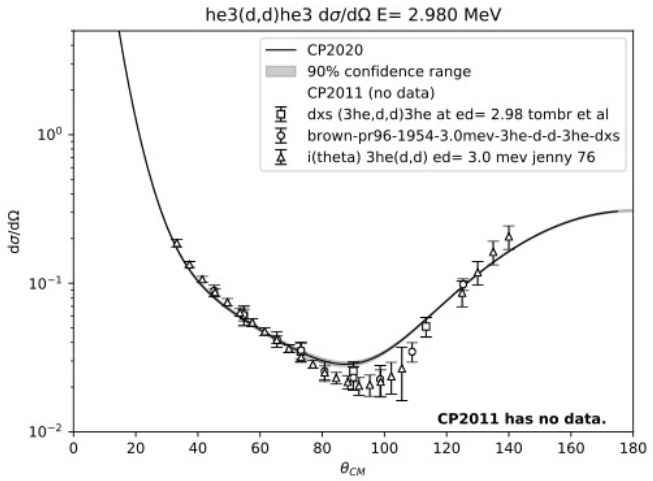
## $^{3}$He(d,d)$^{3}$He



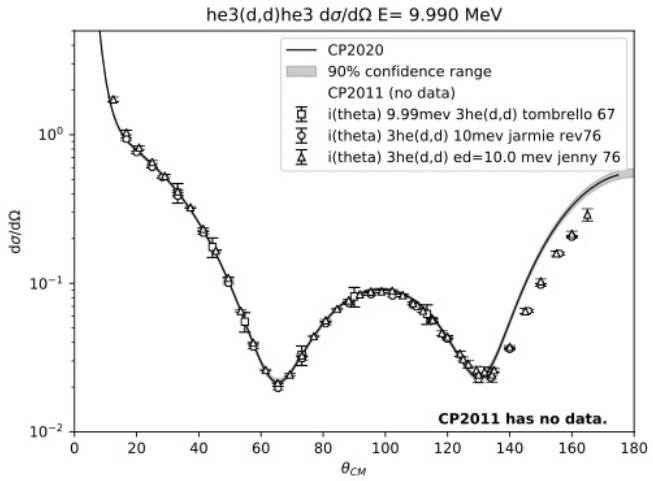

(a)




(b)



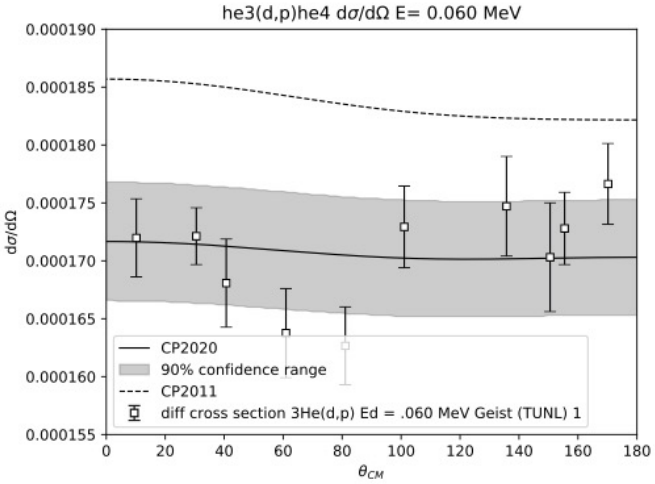

(c)



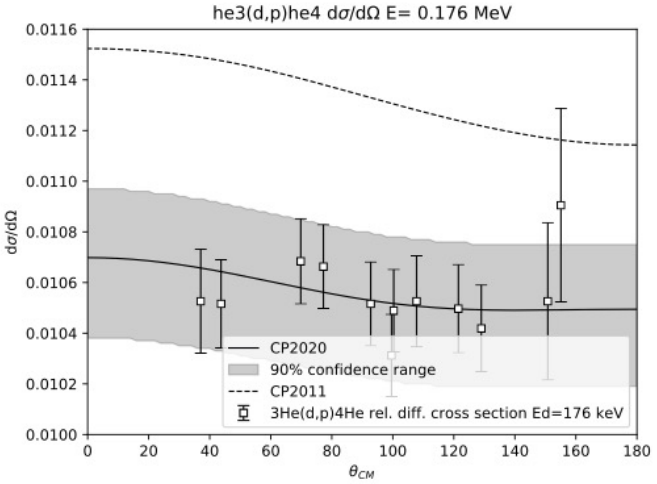

(d)

# $^{5}$Li system evaluation

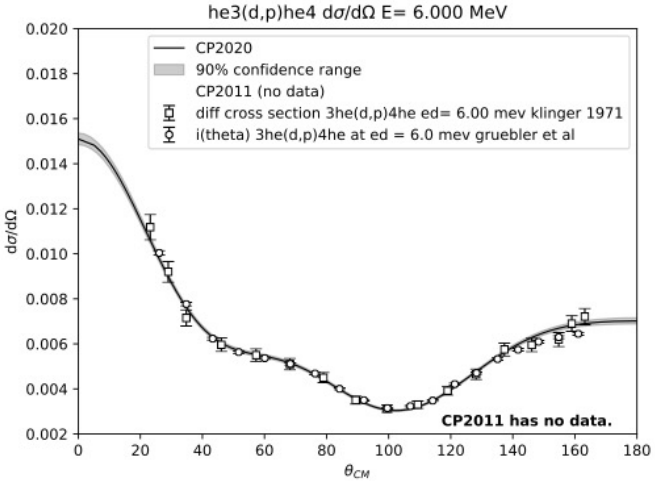
## $^{3}$He(d,p)$^{4}$He



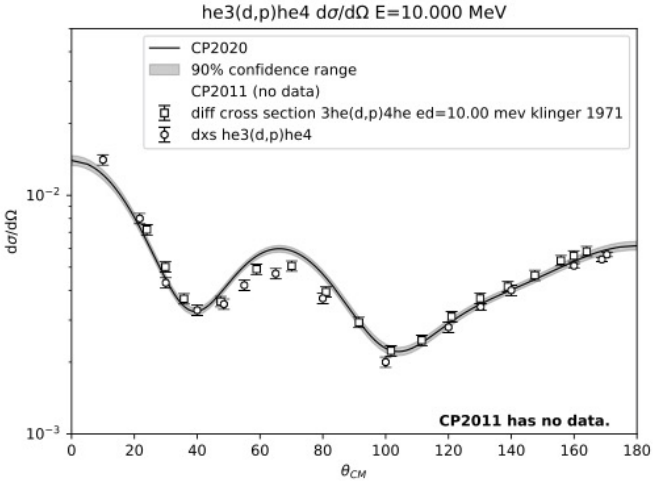

(a)




(b)



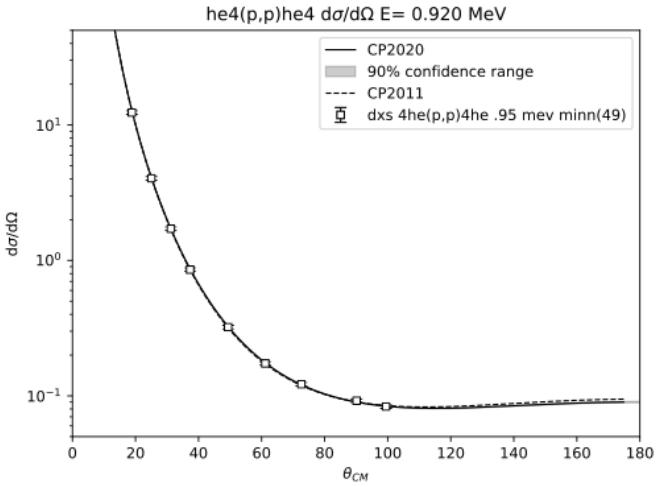

(c)



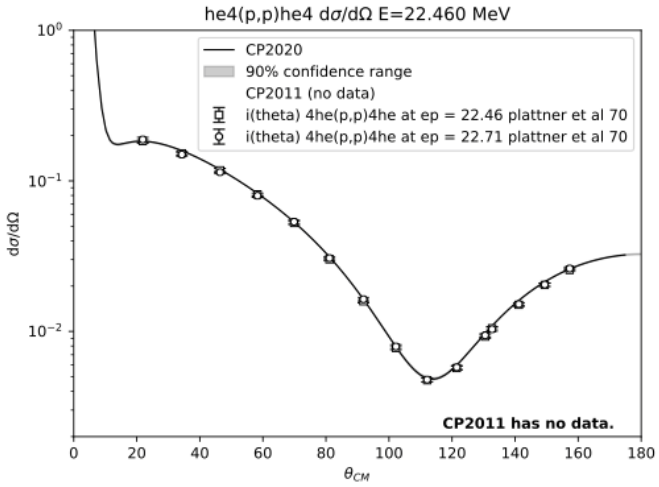

(d)

# $^{5}$Li system evaluation

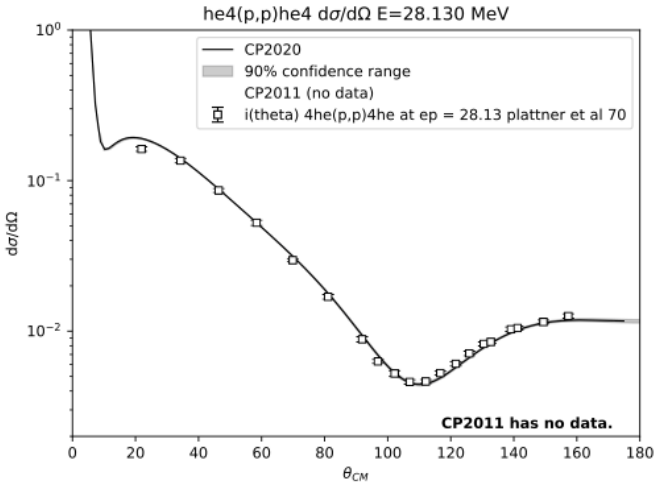
## $^{4}$He(p,p)$^{4}$He



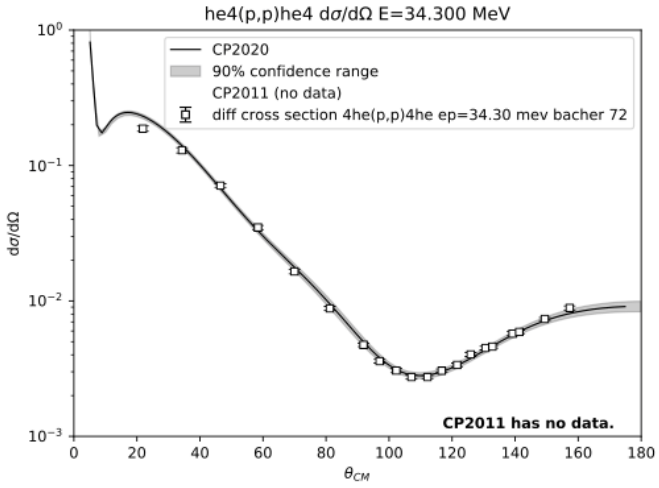

(a)




(b)



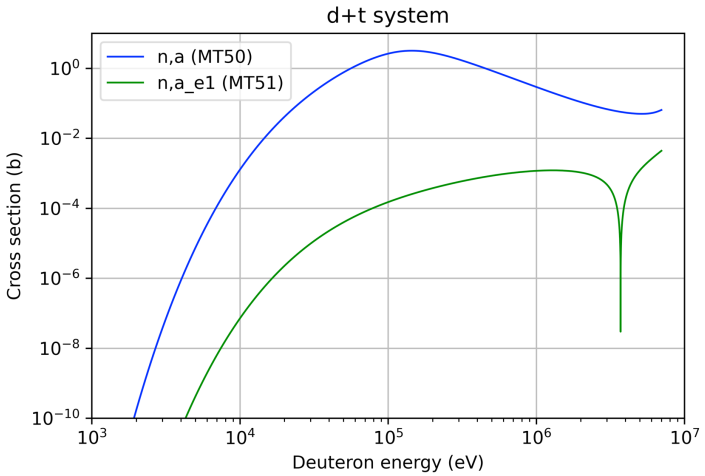

(c)




(d)

# MF2 resonance parameters

- "Full" evaluation
- NJOY test buggy
  - We think we know why…
    - formatting




```
 1.003000+3 2.98959578          0          0          1          0 128 2151
 1.003000+3 1.000000+0          0          0          1          0 128 2151
 1.000000+0 2.000000+7          1          7          0          1 128 2151
 0.000000+0 0.000000+0          1          4         13          0 128 2151
 0.000000+0 0.000000+0          3          0         36          6 128 2151
 1.99625581 2.98959578 1.000000+0 1.000000+0 1.000000+0 5.000000-1 128 2151
 4.172509-7 1.000000+0 1.000000+0 2.000000+0 1.000000+0 0.000000+0 128 2151
 1.000000+0 3.96713130 0.000000+0 2.000000+0 5.000000-1 0.000000+0 128 2151
 17588938.2 1.000000+0 1.000000+0 5.000000+1 1.000000+0 1.000000+0 128 2151
 1.000000+0 3.98821926 0.000000+0 2.000000+0 5.000000-1 0.000000+0 128 2151
-2224575.58 1.000000+0 1.000000+0 5.100000+1 1.000000+0 1.000000+0 128 2151
 1.500000+0 0.000000+0          0          0          6          1 128 2151
 1.000000+0 0.000000+0 1.500000+0-3.700000-1 5.100000+0 5.100000+0 128 2151
 0.000000+0 0.000000+0          0          4         24          4 128 2151
 154389.922-1207.42647-84.7282663-12.5755660-379.896791 0.000000+0 128 2151
 24025435.2 595.728894-1855.95536-558.678031-949.504553 0.000000+0 128 2151
 13219863.4 274.125714-606.067903 1075.57431-227.461704 0.000000+0 128 2151
 48703152.9-610.462073-1512.12218-325.197899 3042.22955 0.000000+0 128 2151
 5.000000-1 0.000000+0          0          0          6          1 128 2151
 1.000000+0 1.000000+0 1.500000+0-3.000000+0 5.100000+0 5.100000+0 128 2151
 0.000000+0 0.000000+0          0          3         18          3 128 2151
 15132068.0-954.248566 61.1518592-204.578201-126.149686 0.000000+0 128 2151
  166773435 803.380352 69.1628993-4577.73718 2603.55979 0.000000+0 128 2151
  166773435 799.264407 474.608977-2095.27865-3568.63138 0.000000+0 128 2151
 2.500000+0 0.000000+0          0          0          6          1 128 2151
 1.000000+0 1.000000+0 1.500000+0-1.000000+0 5.100000+0 5.100000+0 128 2151
 0.000000+0 0.000000+0          0          5         30          5 128 2151
-37941817.8 0.000000+0 0.000000+0-3480.84374 0.000000+0 0.000000+0 128 2151
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  283514840 887.314189 887.725962-6937.97393 2545.49572 7304.64606 128 2151
  100064061-3.609298+3 0.000000+0 0.000000+0 0.000000+0 0.000000+0 128 2151
 7305954.43 0.000000+0 0.000000+0 831.697695-192.163647 807.893837 128 2151
 3.500000+0 0.000000+0          0          0          6          1 128 2151
 1.000000+0 2.000000+0 1.500000+0-1.000000+0 5.100000+0 5.100000+0 128 2151
 0.000000+0 0.000000+0          0          4         24          4 128 2151
```
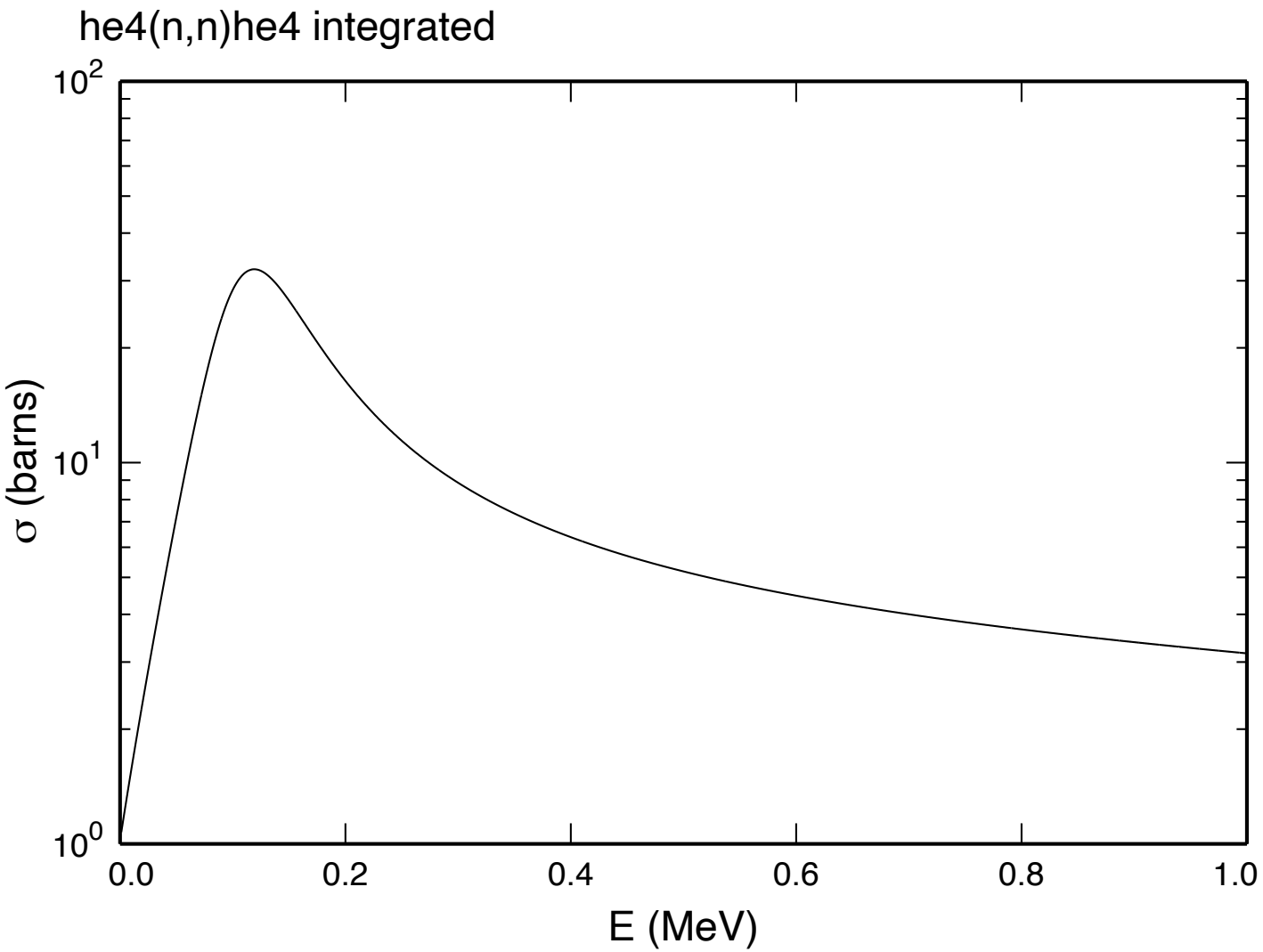

Manual update: revisions for resonance parameters sections

- https://git.nndc.bnl.gov/endf/format/endf6man.git
  - SHA: 56da8d2b

# MF2 resonance parameters

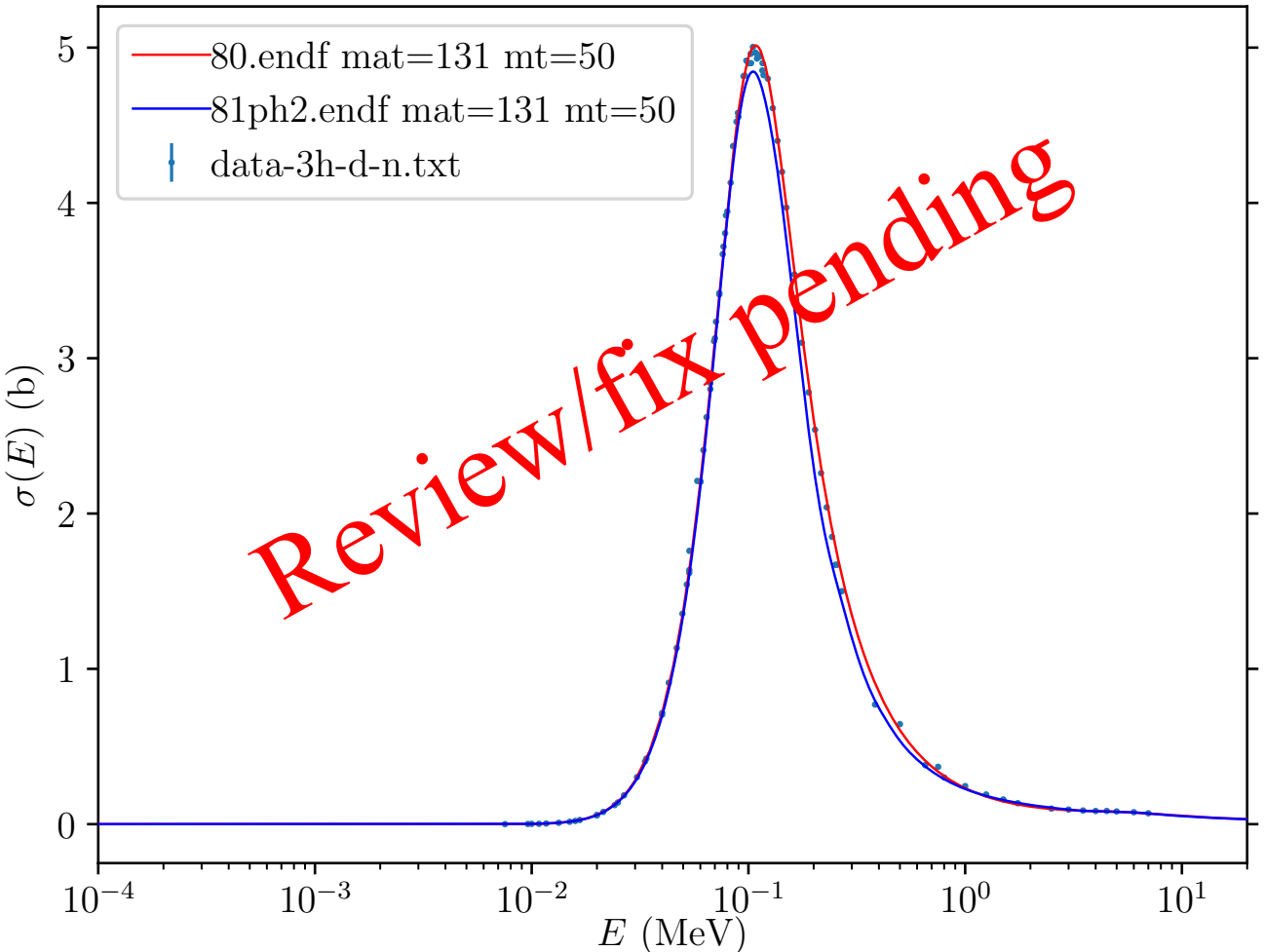
- "Test" evaluation
  - single channel, single resonance



# d+$^3$H

## d-001_H_003.endf

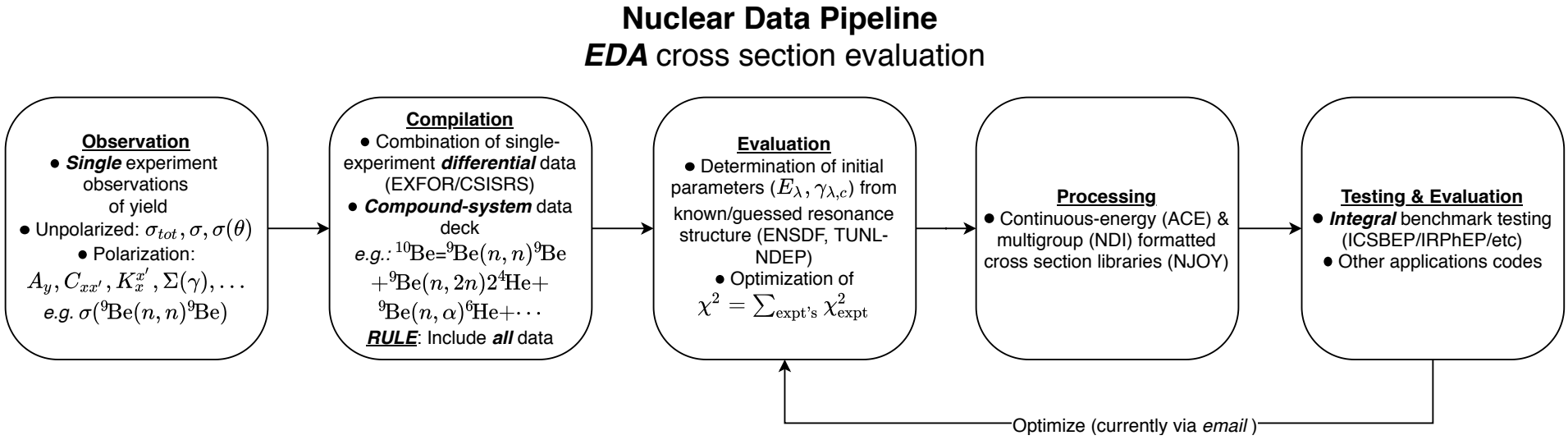
- Questions about the 8.1 repository
  - Is the initial commit 8.0?
    - If not, where did it come from?
  - What is motivating the changes from 8.0?
    - Apparently MT50 is now worse than 8.0:



Thank you!

# Evaluation pipeline

## *EDA R-matrix procedure*




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

# R-matrix

## *Overview of evaluation framework*

Exterior region

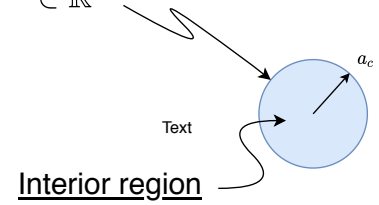
$$|\Psi_c^{(+)}\rangle = |\mathscr{I}_c\rangle - \sum_{c'} S_{cc'}|\mathscr{O}_{c'}\rangle$$

$$S_{cc'} = \delta_{cc'} - 2\pi i \rho_c T_{cc'}$$

$r \to \infty$

Channel surface

$\in \mathbb{R}^{3A-4}$




Interior region

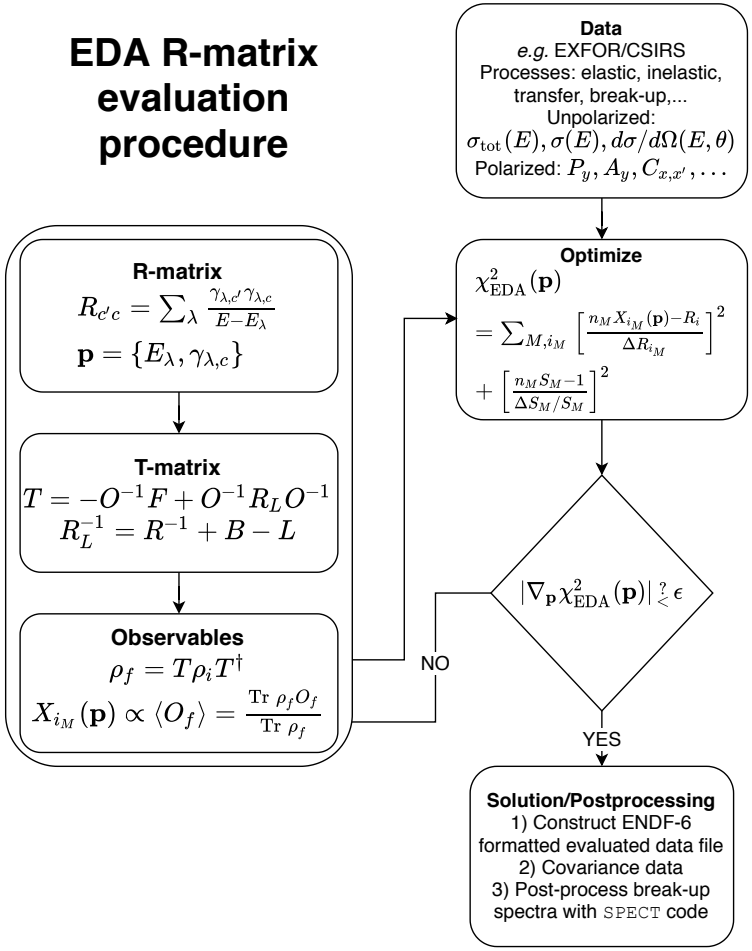
$$[H + \mathscr{L}_B]\,|\lambda\rangle = E_\lambda |\lambda\rangle$$

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

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

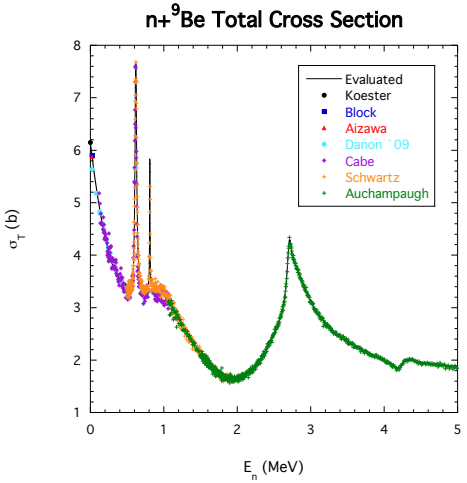
$$R_{B,c'c} = \langle c'|[H + \mathscr{L}_B - E]^{-1}|c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$

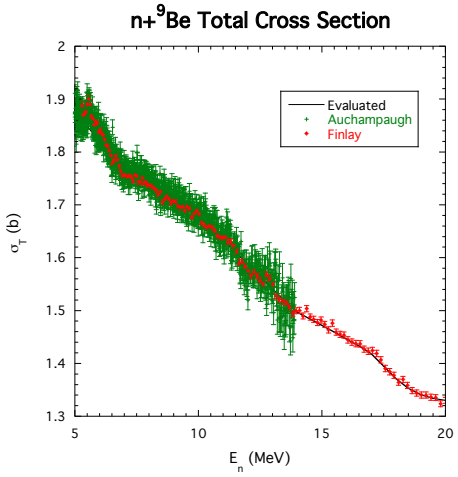
## EDA R-matrix evaluation procedure

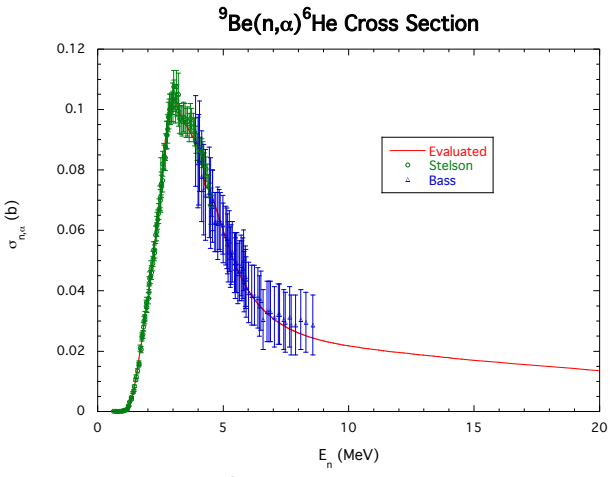


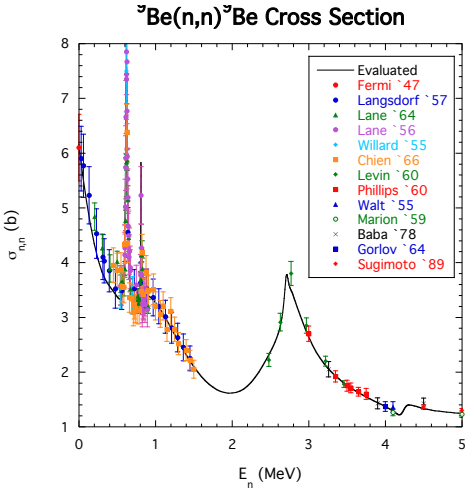
# n+$^{9}$Be

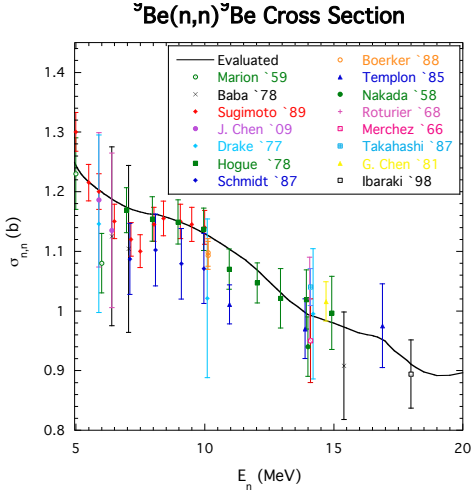
## *Integrated cross sections*

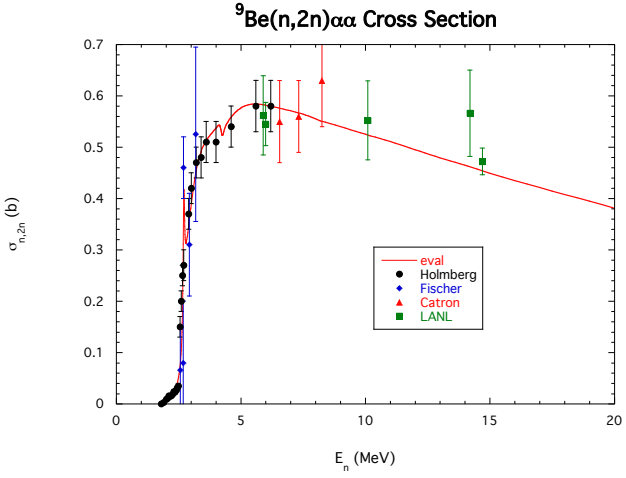


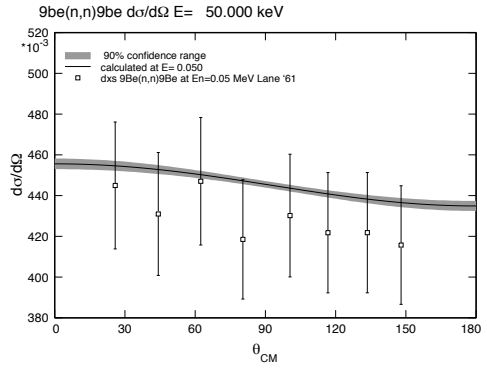



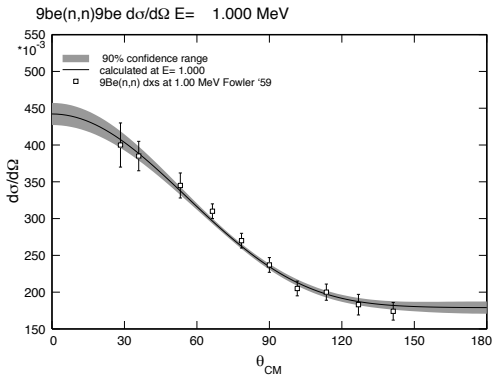



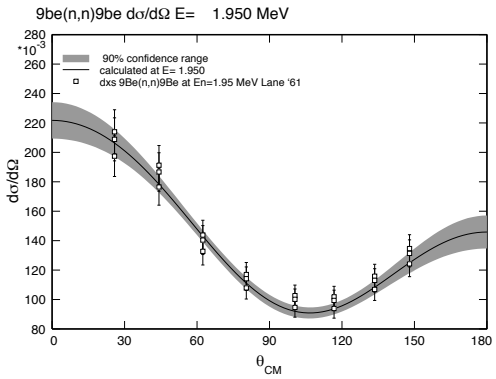



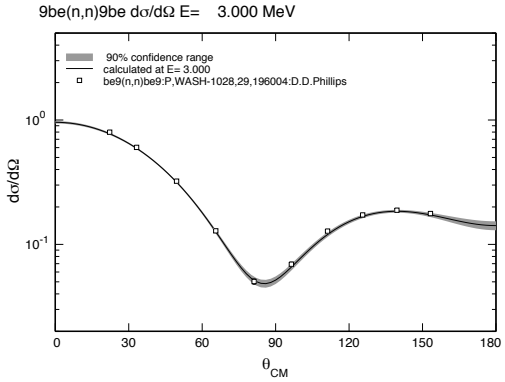
# n+$^{9}$Be

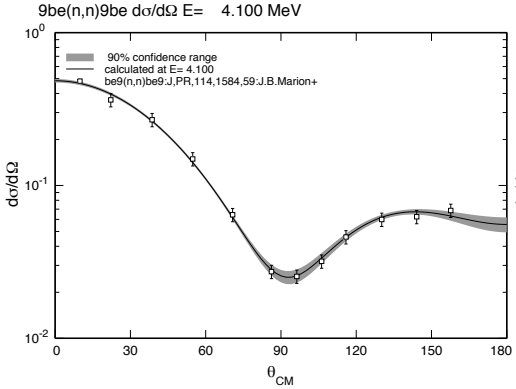
## *Differential cross sections $^{9}$Be(n,n$_0$)$^{9}$Be*

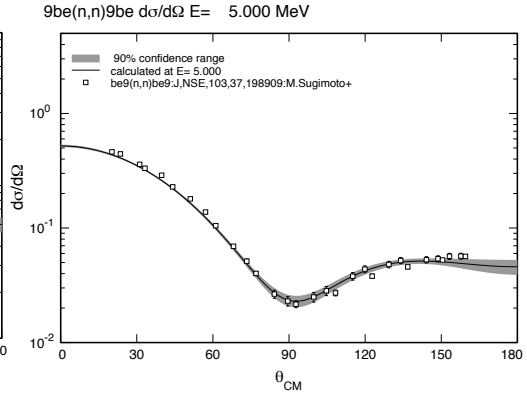


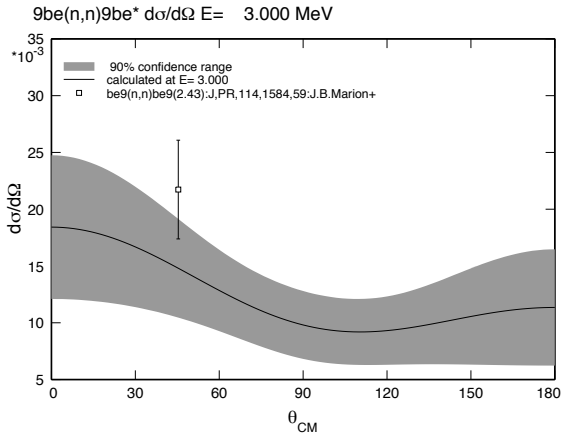



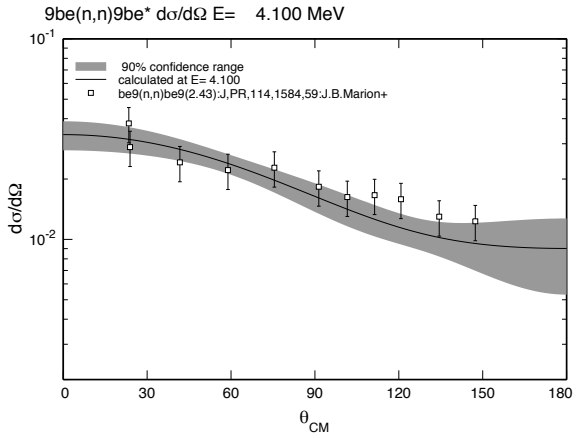



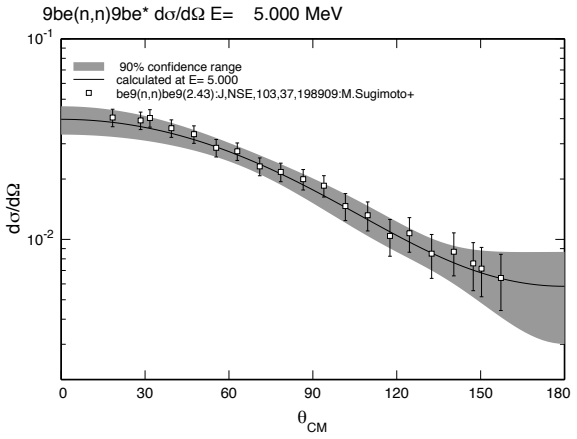



# n+$^{9}$Be

## *Differential cross sections $^{9}$Be(n,n$_1$)$^{9}$Be**




**New Evaluation 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).
- Testing/benchmarking (on slides following n+$^{16}$O)