

# Charged Particle Evaluations

## plans for post - ENDF/B-VIII.0

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November 8, 2017

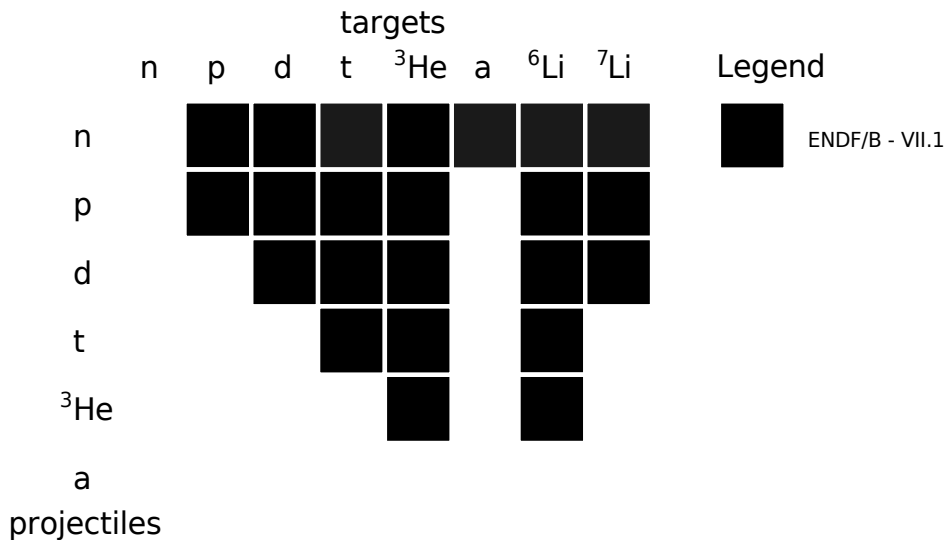


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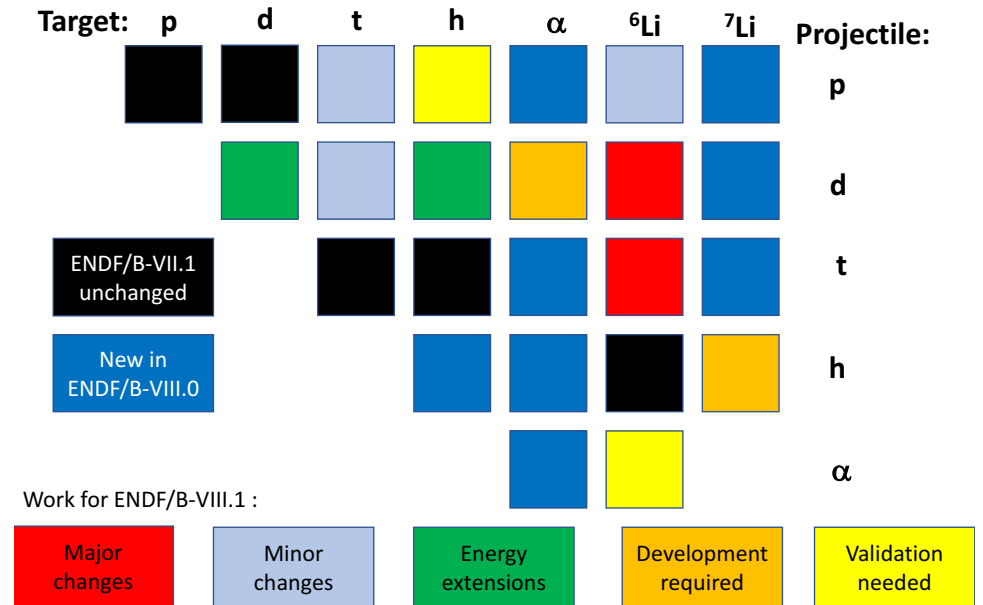
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

# Past, Present and Future Evaluations

## Evaluations in ENDF/B-VII.1



## Evaluations in ENDF/B-VIII.0 and 1



Submitted from LLNL in October 2016:  
 ENDF for a+a, d+<sup>7</sup>Li, h+h, h+a, p+a, p+<sup>7</sup>Li, t+a, t+<sup>7</sup>Li

# Thermonuclear Reaction Library

- Legacy ECPL/ENDL99 evaluations
  - Incident charged particles (p,d,t,He3,He4), light targets  $Z \leq 3$  (p,d,t,He3,He4,Li6,Li7)
  - R.M. White, D.A. Resler, S.I. Warshaw 'Evaluation of Charged-Particle Reactions for Fusion Applications,' Proc. from Nuclear Data for Sci. and Tech., Ed. S.M. Qaim, Juelich, Fed. Rep. Germany, 13-17 May (1991)
  - S.T. Perkins, D.E. Cullen, 'Elastic Nuclear plus Interference cross sections for light-charge particles' Nucl. Sci. Eng. 77, 20-39 (1981)
- 2010 evaluations at LLNL by Petr Navratil, David Brown & Chris Hagmann
  - Main sources for new evaluations
    - Descouvemont R-Matrix analysis
      - P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam, Atomic Data & Nucl. Data Tables 88, 203 (2004)
    - NACRE (Nuclear Astrophysics Compilation of REaction rate)
      - C. Angulo et al., Nucl. Phys. A656 (1999)3-187
    - Experimental data not in EXFOR
- Include also parts from:
  - LANL n+n evaluation by Gerry Hale
  - JENDL-4 n+d, n+He3 evaluations
- All the new evaluations are already in ENDL2011, and tested in applications.



# Major Improvements

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- d+Li6 evaluation
- t+Li6 evaluation

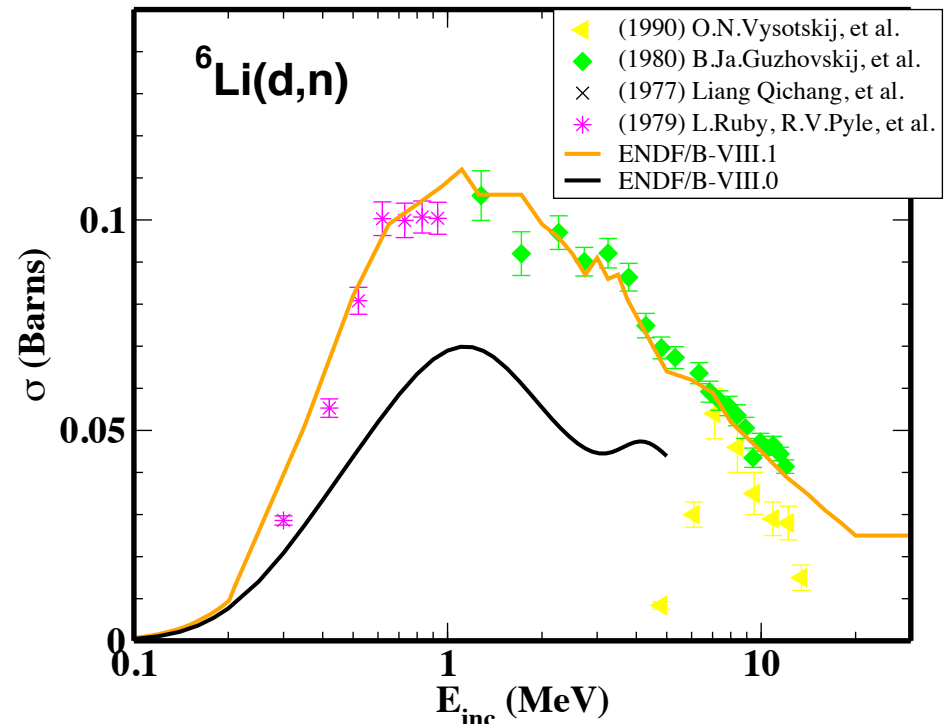
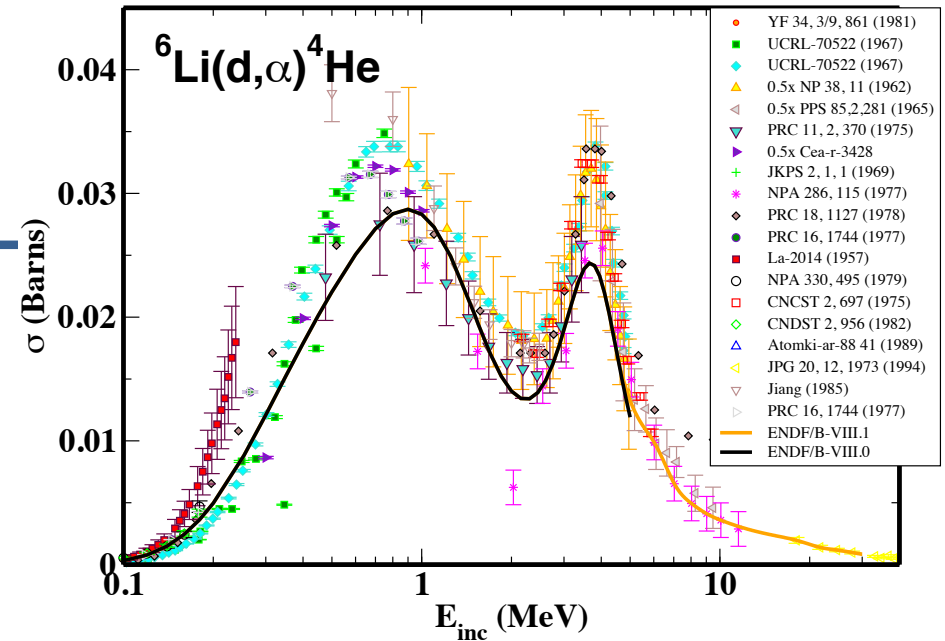


# d+Li6 evaluation

- ENDF/B-VIII.0 (Page 2004)
  - (d,el), (d,n<sub>0</sub>), (d,p<sub>0</sub>), (d,a<sub>0</sub>)
- ENDF/B-VIII.1 (Navratil 2010)
  - (d,el) from ENDF (extended to higher energies)
  - (d,a) from ENDF (up to 4.55 MeV)
    - extended to higher energies to match data from [3,4]
    - ENDF low, needs re-evaluating
  - (d,n+He3) from ECPL

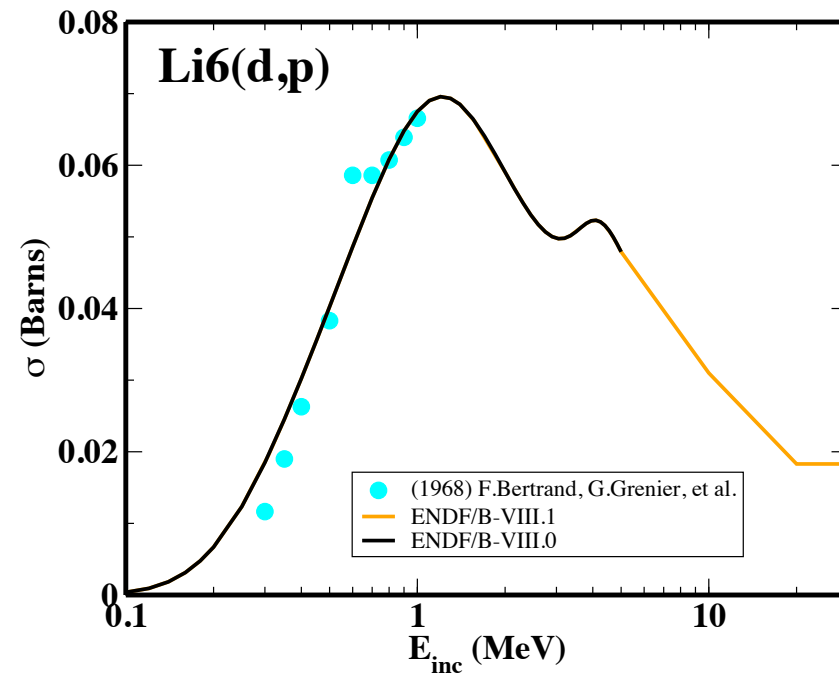
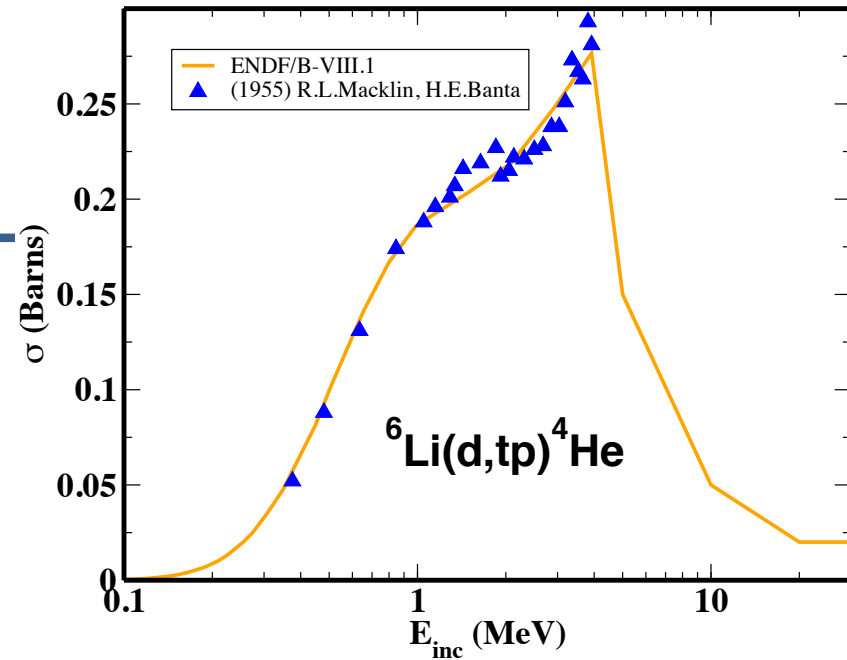
[3] R. Risler, W. Gruebler, A. A. Debenham, V. Koenig, P. A. Schmelzbach, D. O. Boerma, Nucl. Phys. A 286, 115 (1977)

[4] N Arena, I Ya Barit, S Cavallaro, A d'Arrigo, G Fazio, G Giardina, V V Ostashko, M Sacchi, V N Urin and S V Zuyev, J. Phys. G 20, 12, 1973 (1994)



# d+Li6 evaluation

- ENDF/B-VIII.0 (Page 2004)
  - (d,el), (d,n<sub>0</sub>), (d,p<sub>0</sub>), (d,a<sub>0</sub>)
- ENDF/B-VIII.1 (Navratil 2010)
  - (d,n) from ECPL
  - (d,p) from ENDF (extended to higher energies)
  - (d,t+p) from ECPL, expt data labeled as (d,t)

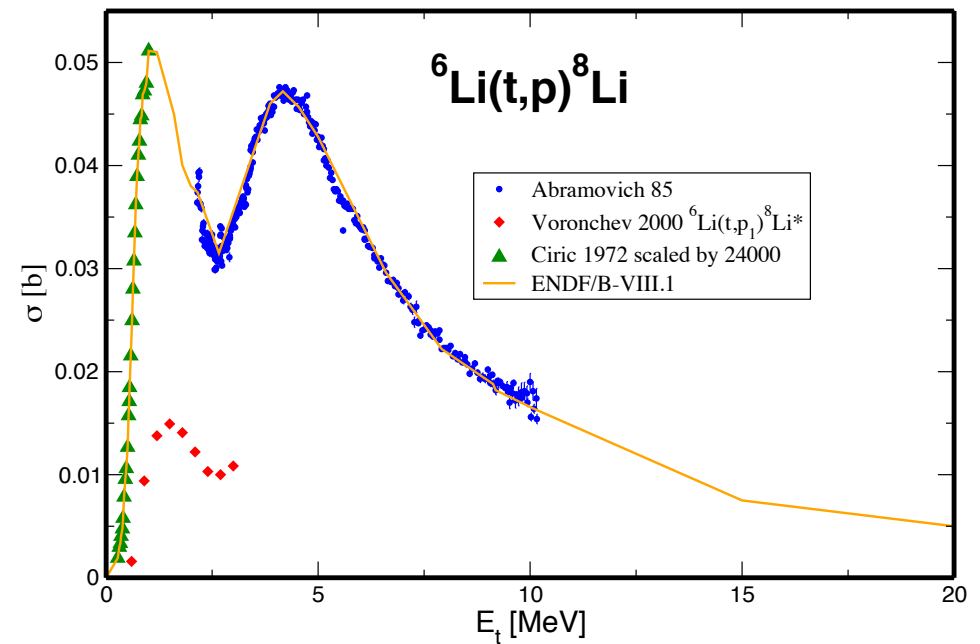
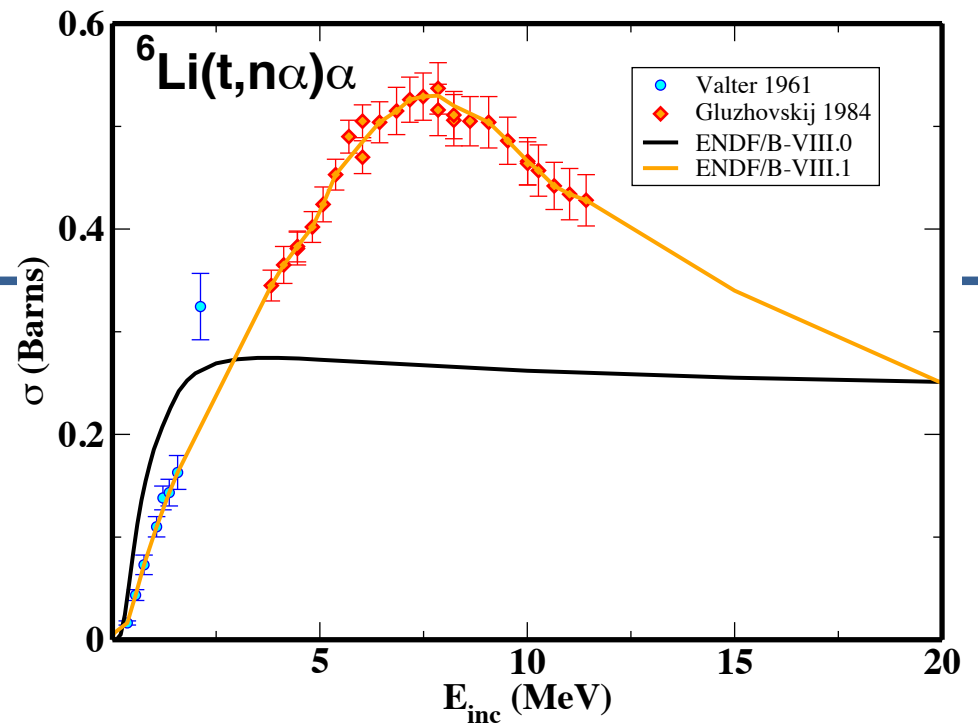




# t+Li6 evaluation

- ENDF/B-VIII.0 (Hale 2001)
  - (t,el), (t,na), (t,d<sub>0</sub>)
- ENDF/B-VIII.1 (Navratil, Brown, Hale 2010)
  - (t,el) from ENDF
  - (t,2n) from ECPL
  - (t,na)
    - Based on data by Valter et al. [3] and Gluzhovskij et al. [4]
    - Angular distributions: From ECPL
  - (t,p)
    - Based on data by Abramovich [7].
    - Un-normalized data by Ciric [6] scaled by 24000 to match [7]
    - Voronchev data [5] for cross section of <sup>8</sup>Li excited state seems to justify existence of peak around 1.5 MeV
    - Angular distributions: proton distribution same as neutron distribution from the (n2a) reaction, ignoring the mass differences
  - (t,d) from ENDF

[3] A.K.Valter, P.I.Vacet, L.Ja.Kolesnikov, S.G.Tonapetjan, K.K.Chernjavskij, A.I.Shpetsyj, Atomnaya Energiya 10, (6), 577 (1961)  
 [4] B.Ja.Guzhovskij, S.N.Abramovich, A.G.Zvenigorodskij, S.V.Trusillo, Prikladnaya Yadernaya, Spektroskopiya 13, 135 (1984)  
 [5] V T Voronchev, V I Kukuljin, J. Phys. G: Nucl. Part. Phys. 26 L123 (2000)  
 [6] D.Ciric, B.Stepancic, R.Popic, D.Stanojevic, M.Aleksic, Fizika, 4, 193, (1972)  
 [7] S.N.Abramovich, B.Ja.Guzhovskij, A.G.Zvenigorodskij, S.V.Trusillo, S.A.Dunaeva, Izv. Rossiiskoi Akademii Nauk, Ser.Fiz. 50, (1), 65 (1986)



# Minor Improvements

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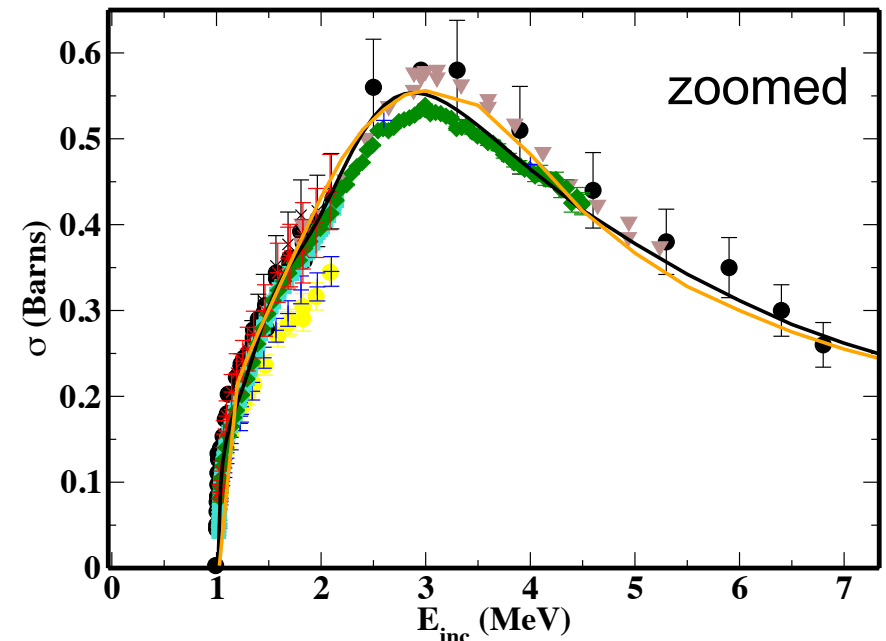
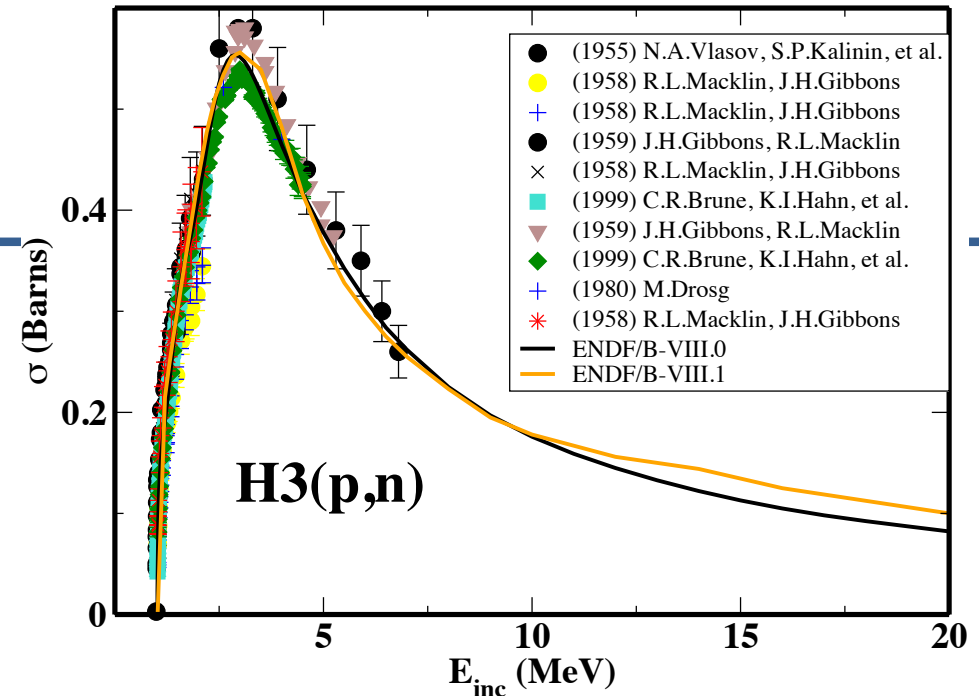
- Better fits within error bars
  - p+H3 evaluation p+t
  - p+Li6 evaluation
  - d+t evaluation
  
- Adding gamma capture channels
  - p+H3 evaluation p+t
  - d+t evaluation





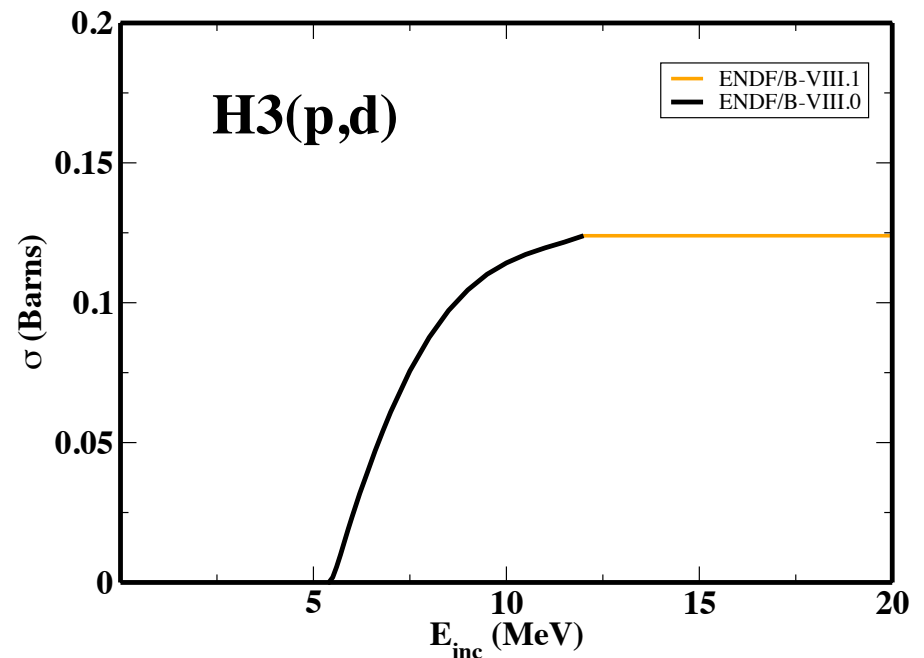
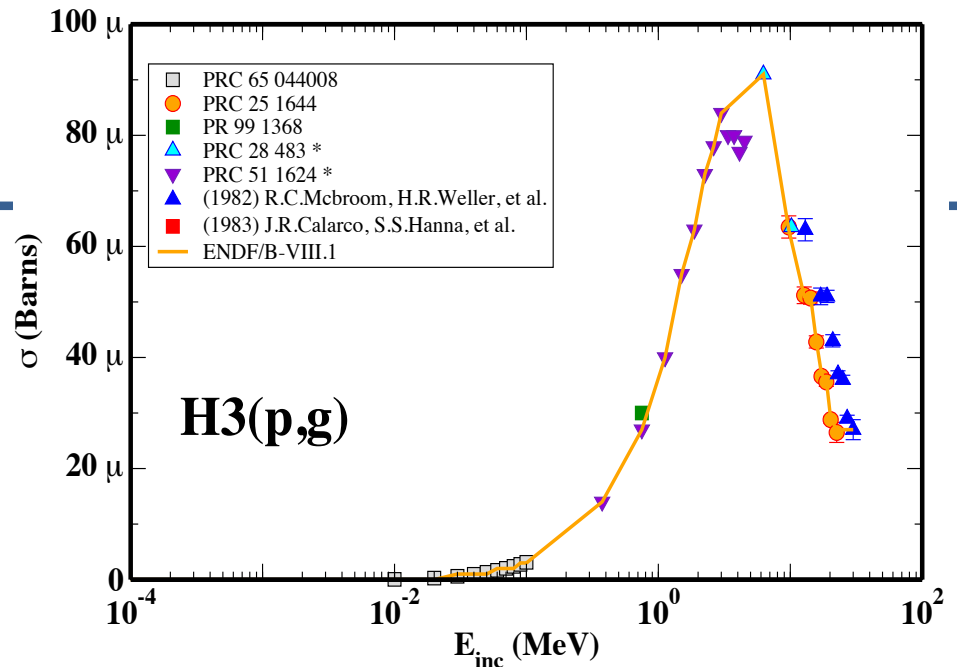
# p+H3 evaluation

- ENDF/B-VIII.0 (Hale 1999)
  - (p,el), (p,n<sub>0</sub>), (p,d<sub>0</sub>) [0-12 MeV]
- ENDF/B-VIII.1 (Navratil et al., 2009)
  - (p,el) from ECPL
  - (p,n<sub>0</sub>) from ECPL (ENDF newer fit with more recent data)
  - (p,d<sub>0</sub>) from ENDF/B-VIII.0
    - An extension to 20 MeV is given for the T(p,n) reaction, based on the inverse of the 3He(n,p) reaction given in the ENDF/B file.
  - (p,g) fit to 5 new data sets from PRC
    - [3] Phys. Rev. C 65: 044008 (2002)
    - [4] McBroom et al., Phys. Rev. C 25, 1644 (1982) [in EXFOR]
    - [5] Phys. Rev. 99, 1368 (1955).
    - [6] Calarco et al., Phys. Rev. C 28, 483 (1983) [EXFOR problem]
    - [7] Phys. Rev. C 51, 1624 (1995)



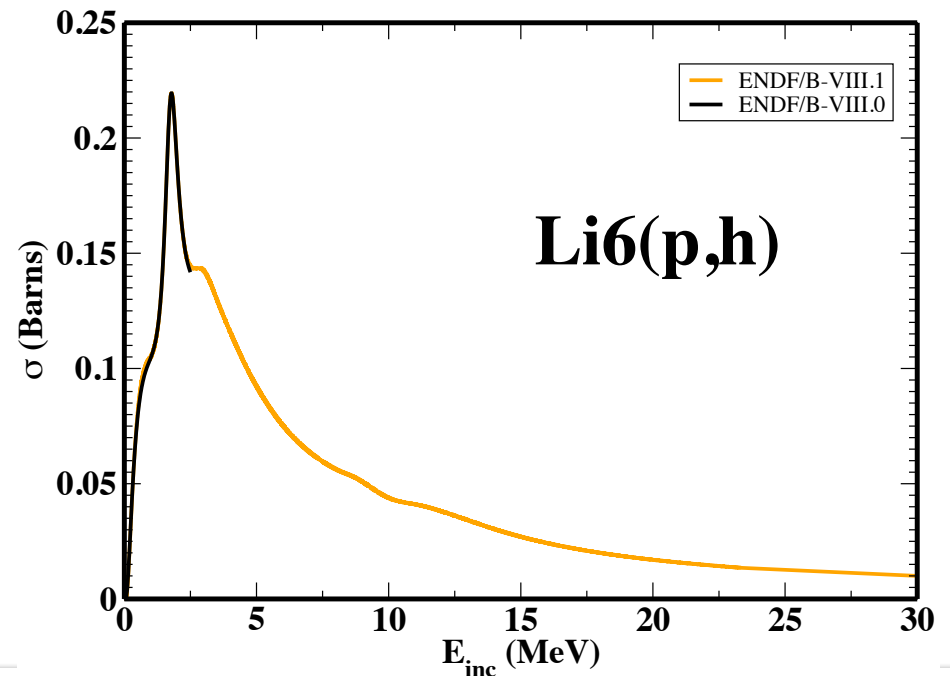
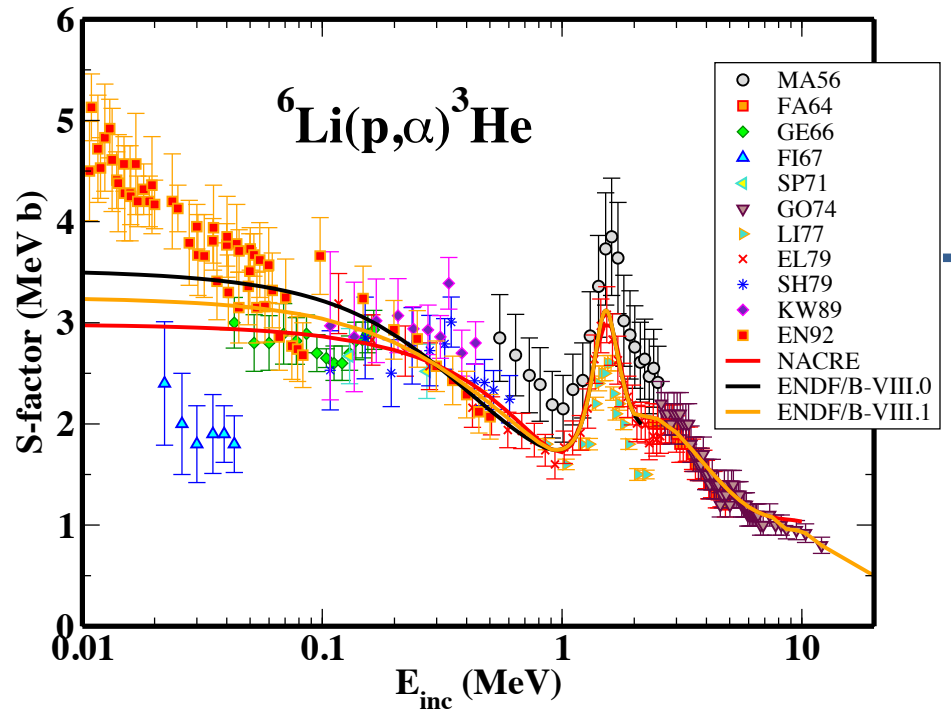
# p+H3 evaluation

- ENDF/B-VIII.0 (Hale 1999)
  - (p,el), (p,n<sub>0</sub>), (p,d<sub>0</sub>) [0-12 MeV]
- ENDF/B-VIII.1 (Navratil et al., 2009)
  - (p,el) from ECPL
  - (p,n<sub>0</sub>) from ECPL (ENDF newer fit with more recent data)
  - (p,d<sub>0</sub>) from ENDF/B-VII.0
    - An extension to 20 MeV is given for the T(p,n) reaction, based on the inverse of the 3He(n,p) reaction given in the ENDF/B file.
  - (p,g) fit to 5 new data sets from PRC
    - [3] Phys. Rev. C 65: 044008 (2002).
    - [4] McBroom et al., Phys. Rev. C 25, 1644 (1982) [in EXFOR]
    - [5] Phys. Rev. 99, 1368 (1955).
    - [6] Calarco et al., Phys. Rev. C 28, 483 (1983) [EXFOR problem].
    - [7] Phys. Rev. C 51, 1624 (1995).



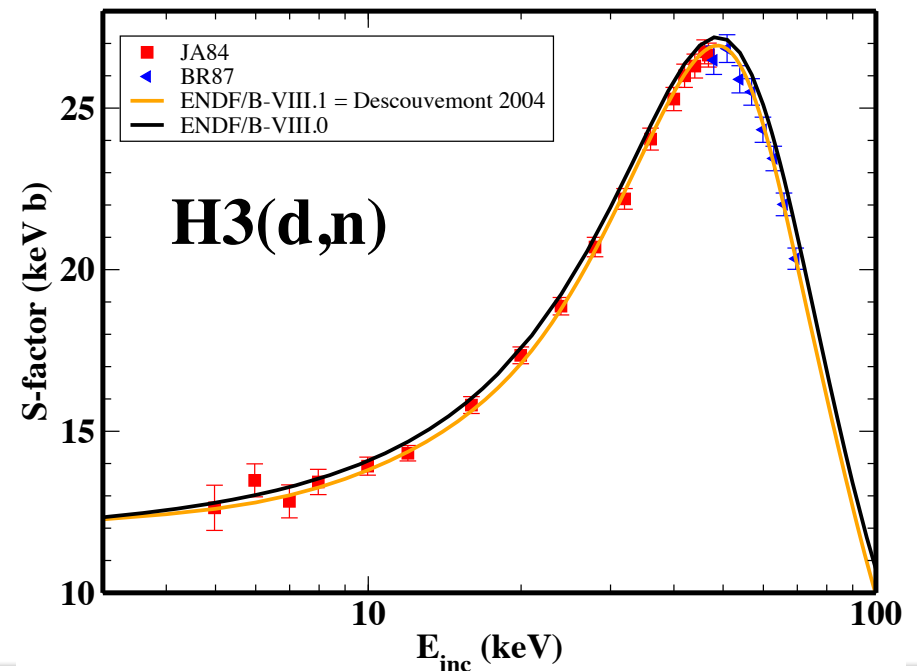
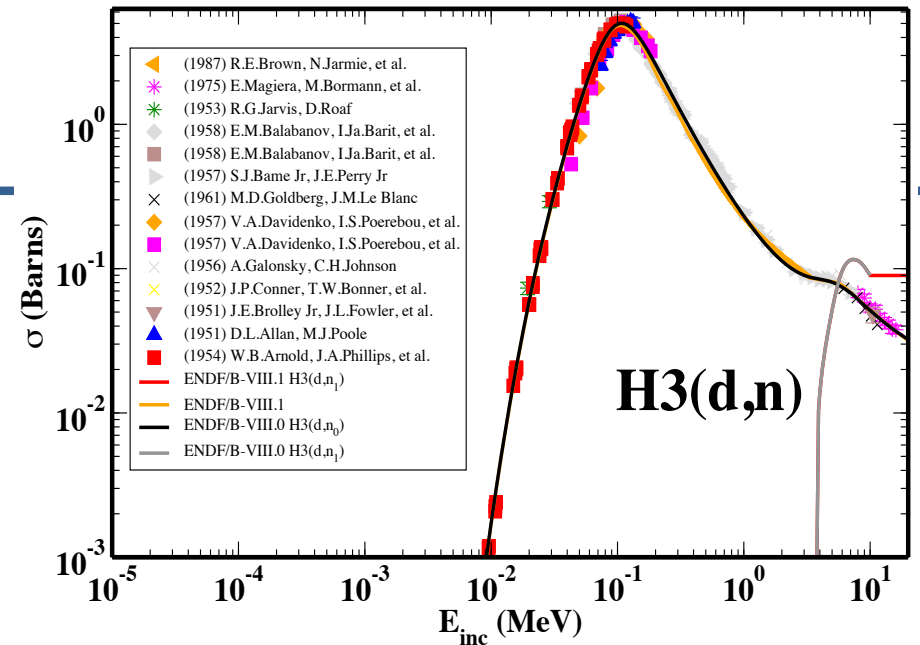
# p+Li6 evaluation

- ENDF/B-VIII.0 (Hale 2001)
  - R-matrix analysis of reactions in the A=7 system, which included data for the  $6\text{Li}(p,p)$  and  $6\text{Li}(p,3\text{He})$  reactions at energies up to about 2.5 MeV.
  - (p,e), (p,He3)
  
- ENDF/B-VIII.1 (Navratil et al. 2010)
  - (p,e) from ECPL and ENDF
  - (p,He3) cross section from Hale, NACRE and Gould
    - 0 - 0.9 MeV average of NACRE [2] and Hale S-factors
    - 0.9 - 2 MeV, Hale S-factor
    - 2 - 7.5 MeV, NACRE S-factor
    - 8 MeV - 12 MeV, S-factor data from [3]
    - 12 MeV - 30 MeV, extrapolation
  - Angular distributions: From ECPL.
  
- NACRE
  - [2] C. Angulo et al., Nucl. Phys. A656 (1999)3-187.
  
- [3] C. R. Gould, R. O. Nelson, J. R. Williams, J. R. Boyce, "Cross-Section Requirements for Charged-Particle Fusion Reactors: The  $6\text{Li}(p,3\text{He})\alpha$  Reaction." Nucl. Sci. Eng. 55 (1974) 267



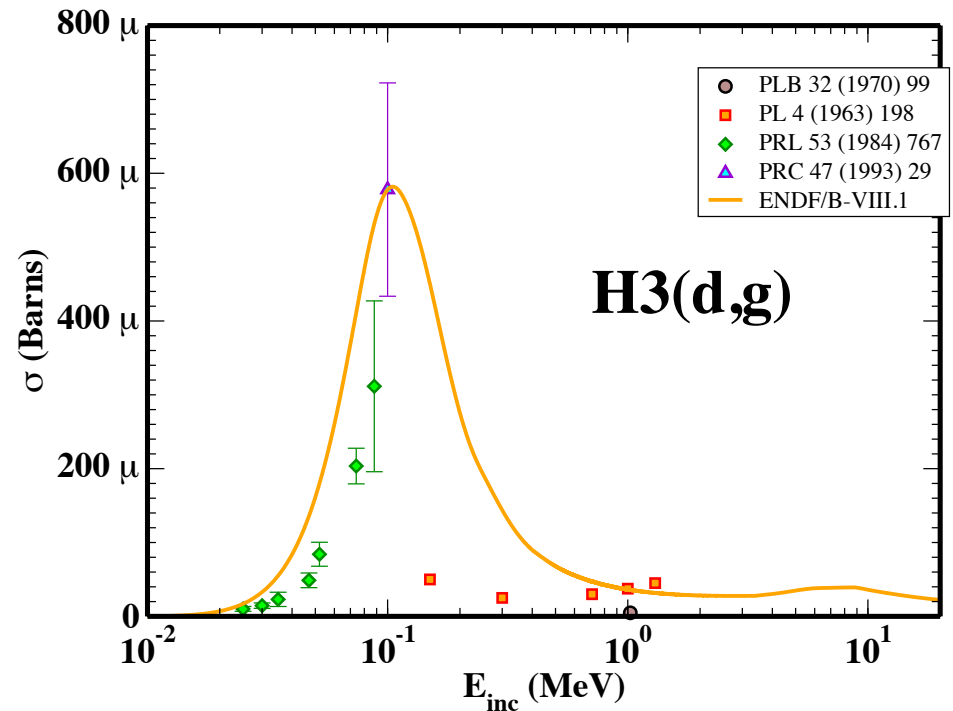
# d+t evaluation

- ENDF/B-VIII.0 (Hale 1995)
  - (d,el), (d,n<sub>0</sub>), (d,n<sub>1</sub>)
- ENDF/B-VIII.1 (Navratil 2009)
  - (d,el) from ECPL
  - H<sub>3</sub>(d,n<sub>0</sub>)
  - Cross-section:
    - Low energy Descouvemont [3]
    - High energy ECPL
    - Peak at 105 keV of 4.85 b
    - TUNL evaluation peak 4.88 b at 105 keV
    - ECPL 4.99 b at 107 keV
    - ENDF 5.01b at 108 MeV
  - Angular distributions: Taken from ECPL
  - H<sub>3</sub>(d,n<sub>1</sub>)He<sub>4</sub>\* → p+t
    - ENDF evaluation extended up to 30 MeV
- Descouvemont 2004
  - [3] P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam Atomic Data and Nuclear Data Tables 88, 203 (2004)
- [4] Nucl. Phys. A 192 (1972) 609



# d+t evaluation

- ENDF/B-VIII.0 (Hale 1995)
  - (d,el), (d,n<sub>0</sub>), (d,n<sub>1</sub>)
- ENDF/B-VIII.1 (Navratil 2009)
  - d + t -> g + 5He\* -> g + n + 4He
  - Cross-section
    - The t(d,g) evaluation is based on Ref. [4]. Several experiments agree that the cross-section ratio is constant at resonance. At higher energies, the ratio appears to rise. In particular, there is a Caltech measurement going up to 9 MeV. Therefore, we did the following:
    - Below 0.4 MeV, we took the ratio  $1.2 \times 10^{-4}$  from the above Ref. [4]
    - From 0.4 to 9 MeV we assumed a linear increase up to  $7 \times 10^{-4}$  according the Caltech data referenced in the above Ref. [4]
    - At higher energies, there is no information. Therefore, we kept the 9 MeV ratio also beyond
    - Note that the EXFOR files with the PRL 53, 767 (84) data appear to be incorrect
  - Angular distributions: Taken from ECPL



# Extensions to higher projectile energies

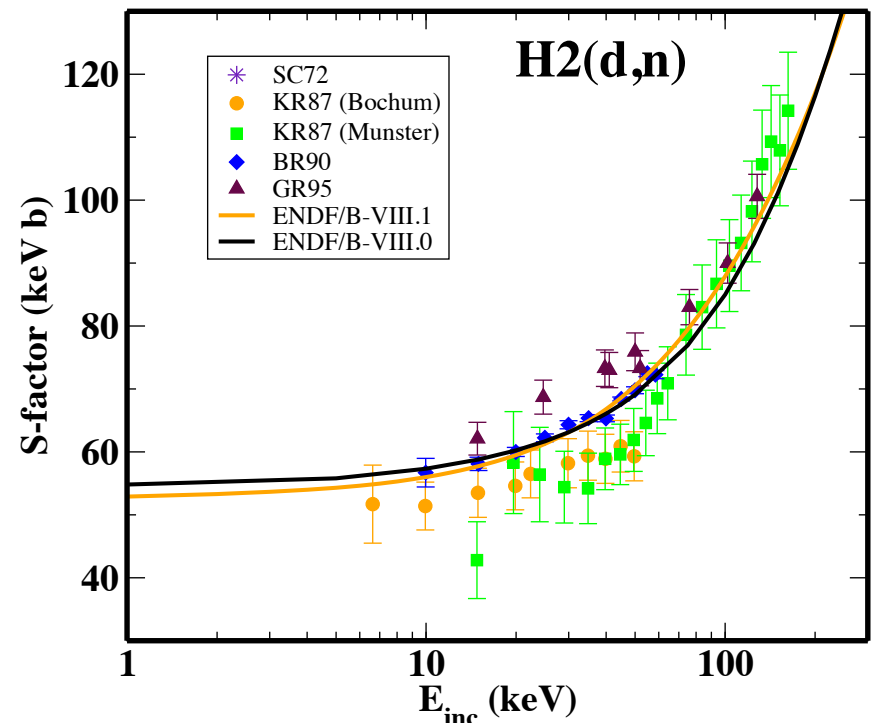
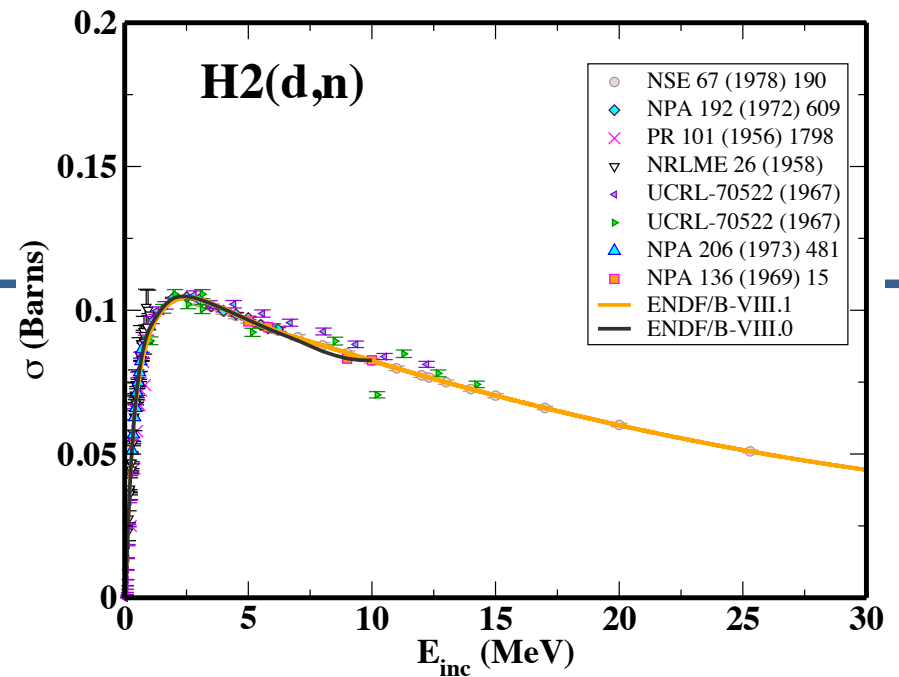
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- d+d evaluation
- d+He3 evaluation    d+h



# d+d evaluation

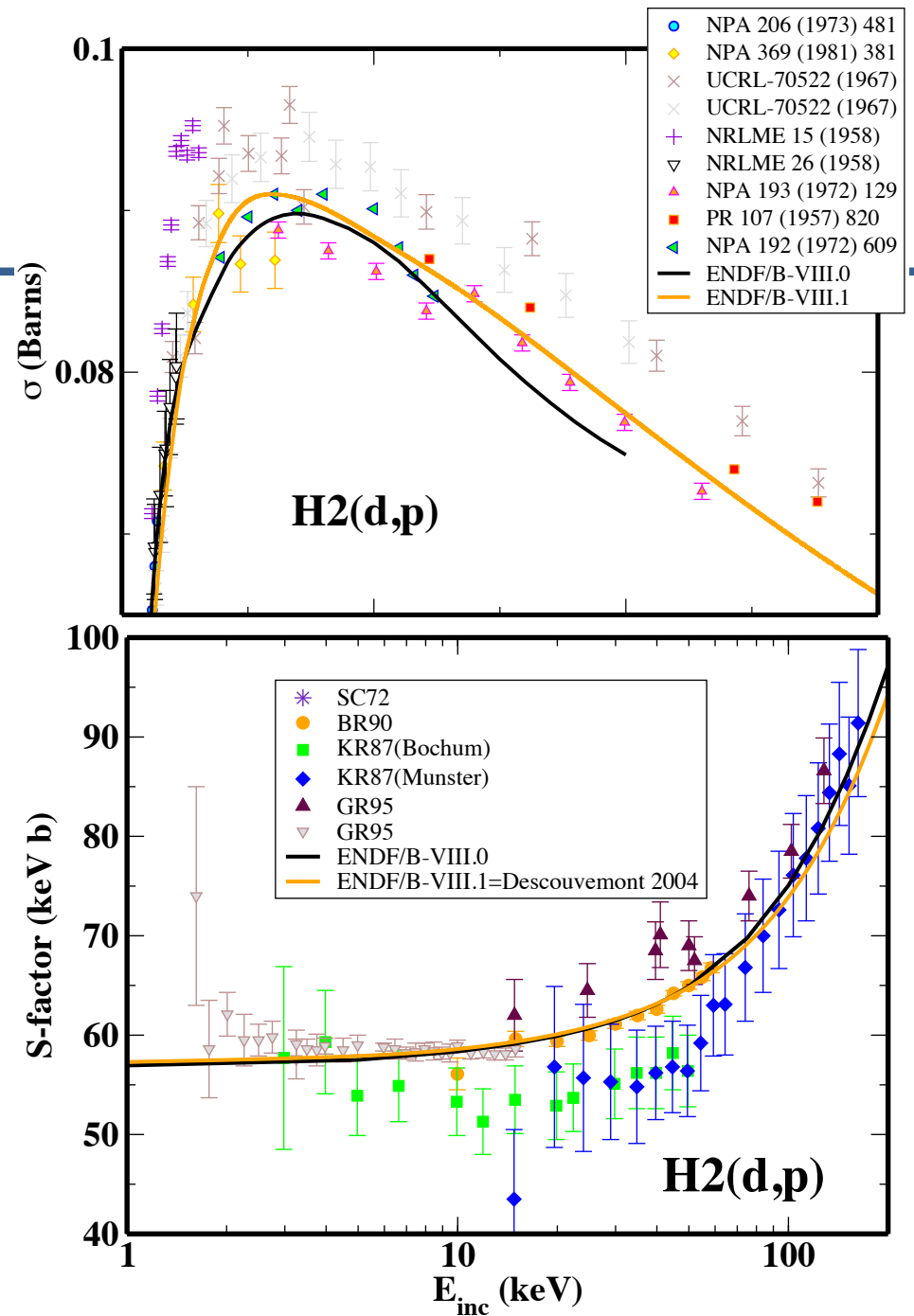
- ENDF/B-VIII.0 (Hale 2001)
  - (d,el), (d,n), (d,p)
  
- ENDF/B-VIII.1 (Navratil 2009)
  - (d,el) from ECPL
  - H2(d,n) and H2(d,p)
  - Cross-section:
    - < 1.96 MeV Descouvemont [3] S-factor R-matrix
    - 1.96 - 5 MeV spline to Ref [4]
    - > 5MeV ECPL
  - Angular distributions: From ECPL
  - Note: The slight mass differences between the p & n and between the t & 3He were ignored in the creation of the angular distributions in ECPL
  
- Decouvemont 2004
  - [3] P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam Atomic Data and Nuclear Data Tables 88, 203 (2004)
  
- [4] Nucl. Phys. A 192 (1972) 609





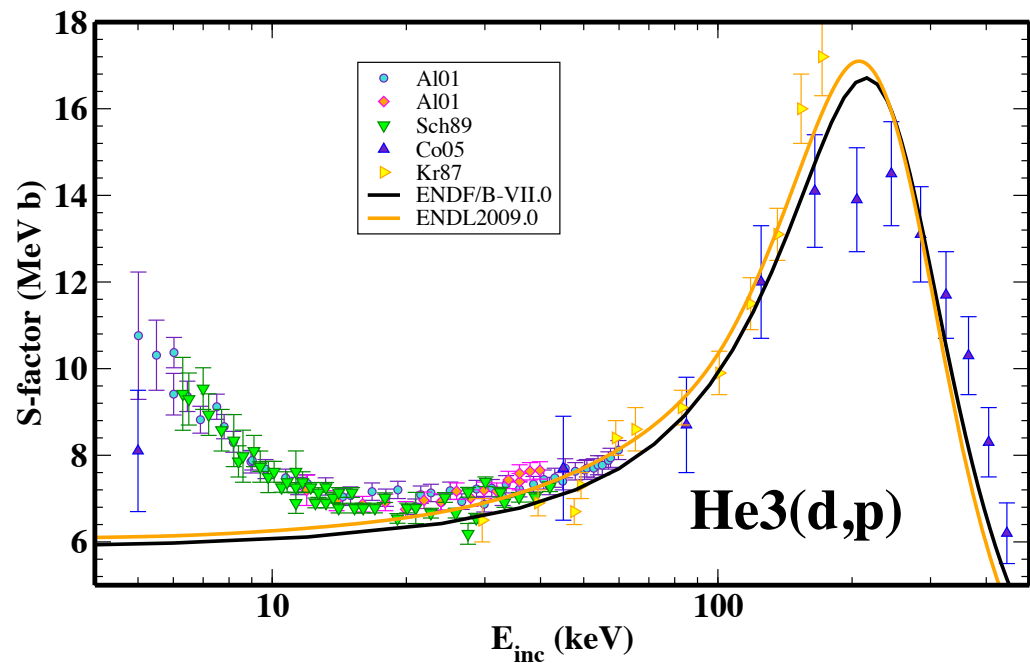
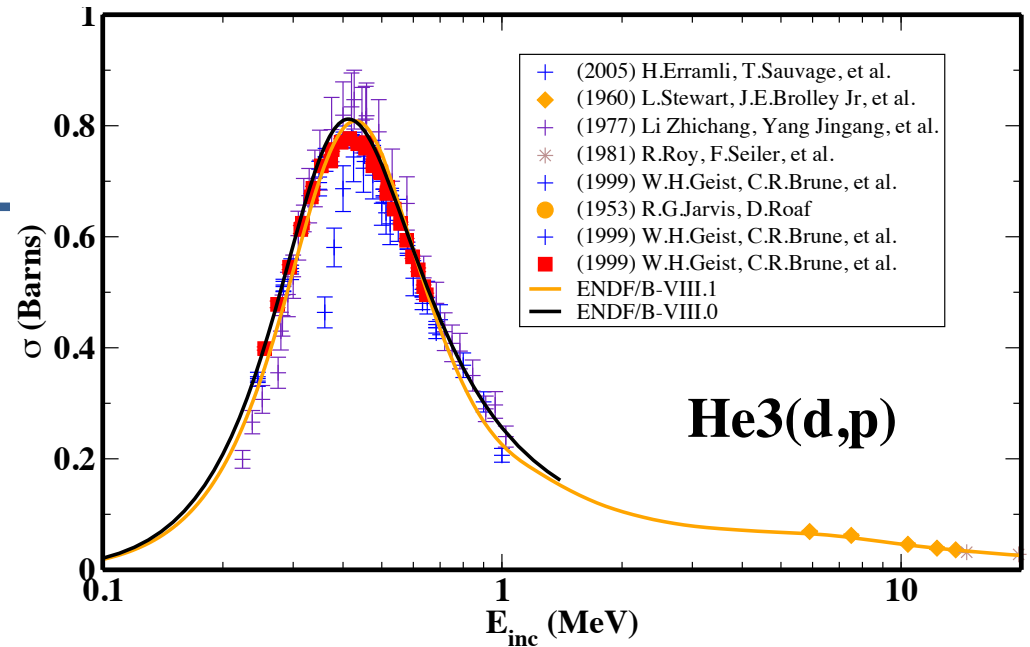
# d+d evaluation

- ENDF/B-VIII.0 (Hale 2001)
  - (d,el), (d,n), (d,p)
- ENDF/B-VIII.1 (Navratil 2009)
  - (d,el) from ECPL
  - H2(d,n) and H2(d,p)
  - Cross-section:
    - < 1.96 MeV Descouvemont [3] S-factor R-matrix
    - 1.96 - 5 MeV spline to Ref [4]
    - > 5MeV ECPL
  - Angular distributions: From ECPL
  - Note: The slight mass differences between the p & n and between the t & 3He were ignored in the creation of the angular distributions in ECPL
- Descouvemont 2004
  - [3] P. Descouvemont, A. Adahchour, C. Angulo, A. Coc, E. Vangioni-Flam Atomic Data and Nuclear Data Tables 88, 203 (2004)
- [4] Nucl. Phys. A 192 (1972) 609



# d+He3 evaluation

- ENDF/B-VIII.0 (Hale 2001)
  - (d,el), (d,p<sub>0</sub>)
- ENDF/B-VIII.1 (Navratil 2009)
  - (d,el) from ECPL
  - He3(d,p)
  - Cross-section:
    - low energy coming from Descouvemont 2004
    - matched at higher energies with ECPL
  - Angular distributions: From ECPL
    - Note: The slight mass differences between the p & n and between t & 3He were ignored in the creation of the angular distributions in ECPL



# Remaining Issues: Development required

- Gamma decay of  ${}^6\text{Li}(3^+)$  resonance, after  $h + {}^7\text{Li}$  reaction
  - Translate to ENDF MT=801, and convert  $\gamma$ -distribution to lab frame
- Gamma decay of  ${}^5\text{He}^*$  resonance, during  $d + t$  reaction
  - Translate to ENDF MT=91 (inclusive  $n^*$ ), with lab distributions for  $n, \text{He4}, \gamma$
- Three-body breakup of deuteron after  $d + \alpha$  reaction
  - 2-steps via  $p + \{ {}^5\text{He} = \alpha + n \text{ resonance} \}$ 
    - Translate to ENDF MT=600, with LRP=1 for  $n$  and  $\text{He4}$
  - 2-steps via  $n + \{ {}^5\text{Li} = \alpha + p \text{ resonance} \}$ 
    - Translate to ENDF MT=50, with LRP=1 for  $p$  and  $\text{He4}$
  - Direct 3-body decay to  $\alpha + n + p$  (no resonances)
    - Translate to ENDF MT=28, MF=3 and 6



# Future Evaluations

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Use full R-matrix evaluations!!

- If possible, publish R-matrix evaluations from LANL
  - Include all R-matrix parameters
  - Include all fitted data normalization factors
- Convert from EDA format (also AZURE, RAC, FRESCO, SAMMY, HYRMA) to GNDS and then ENDF
  - Using my code Ferdinand.py
  - This is being developed with USNDP funding.
- Then can encourage, monitor and verify new R\_matrix fits to data
  - Determine how to fit data above 3-body thresholds
  - Supplement with Hauser-Feshbach models above resonance region
- International effort through IAEA to verify and validate the above R-matrix codes.
  - Marco Pigni explained this in his earlier talk, and showed examples.





**Lawrence Livermore  
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