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Title: Nuclear Data Evaluation Highlights

Author(s): Kawano, Toshihiko; Lovell, Amy Elizabeth; Herman, Michal W.; Mumpower, Matthew Ryan; Paris, Mark W.; Hale, Gerald M.; Stetcu, Ionel

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Nuclear Data Evaluation Highlights

T. Kawano, A. Lovell, M. Herman, M. Mumpower,
M. Paris, G. Hale, I. Stetcu
Theoretical division, T-2

2022 MCNP® User Symposium

Materials & reactions of interest

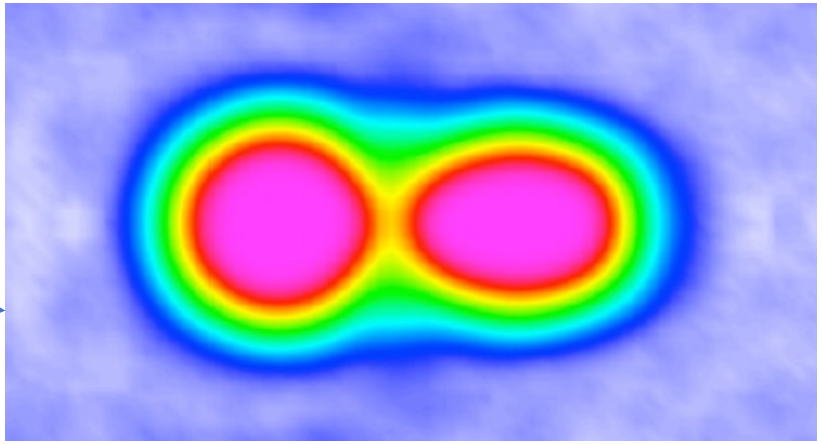
Overview & Motivation

Reactions	Applications
Actinides – (n,g): DANCE – (n,f): DANCE/chi-nu/SPIDER – (g,x)	– Stockpile stewardship [weapons] – Criticality safety [reactors] – Basic science [nuc-astro (r-process)]
Medium mass – ^{58}Ni: LENZ – ^{35}Cl(n,p): LENZ	– Nuclear energy – Structural materials – Diagnostics
Light elements – ^{12,13}C(n,z) & ^{16}O(n,z): LENZ – ^{6}Li(n,z): NZ	– Stockpile stewardship – Structural materials & Diagnostics – Fusion energy/basic science

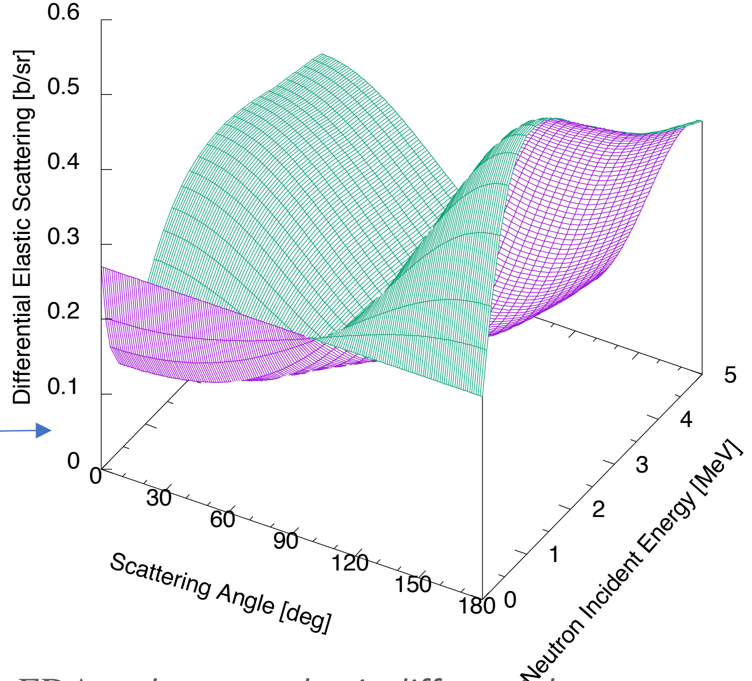
State-of-the-art Theoretical Modeling

Model & evaluation approaches; LANL codes

- **CoH$_3$**: Coupled-channels & Hauser-Feshbach code
  - Optical models; compound reaction; pre-equilibrium; direct capture; FRDM mean-field + Hartree-Fock
- **CGMF**: Cascading Gamma-ray Multiplicity for Fission
  - Monte Carlo Hauser-Feshbach statistical theory
    - Emitted-particles correlation; average properties
    - PFNS, $\bar{\nu}$, gamma multiplicity M_γ, etc.
- **BeoH**: Deterministic implementation of CGMF
  - Delayed quantities, cumulative yields, photofission (new)
- **LISE**: Time-dependent density functional theory
  - HPC TDDFT for superfluid nuclei; Average FF properties
- **EDA$_{f90}$**: relativistic multichannel unitary R-matrix
- Machine Learning/Quantum computing
  - ML: Mixture Density Networks for FF uncertainty quantification
  - QC: Exploratory applications to nuclear shell model



LISE simulation of the time evolution of the fissioning nucleus from a compact shape to two separated fragments. The neutron density is shown at an instance of almost full separation.



EDA$_{f90}$ *deuteron elastic differential cross section*

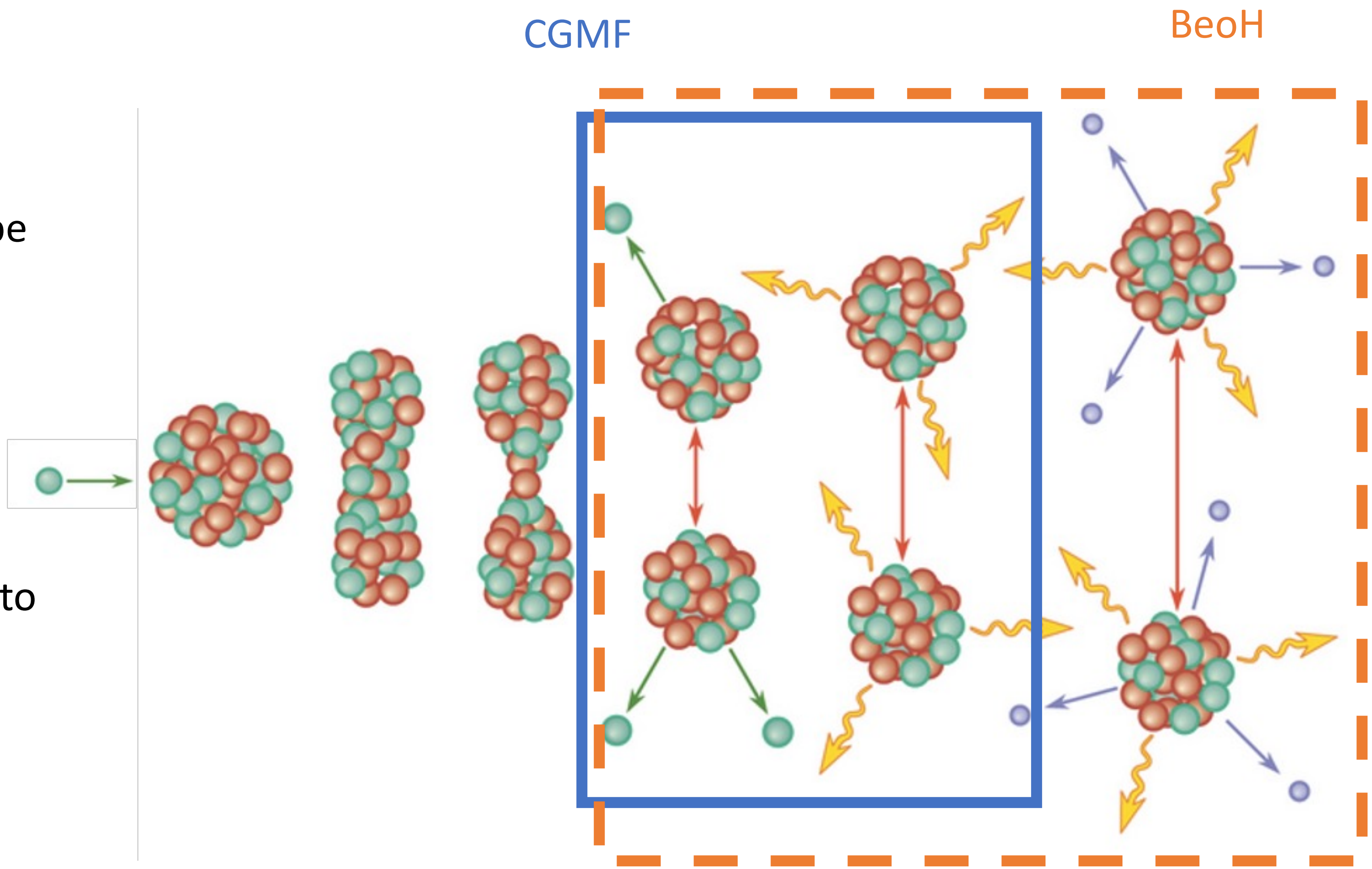
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

CGMF and BeoH consistently calculate prompt/delayed fission observables

CGMF and BeoH both begin with equivalent initial conditions for the fission fragments, so delayed observables calculated with BeoH can be connected back to prompt correlations from CGMF.

CGMF exactly takes into account multi-chance fission (Monte Carlo).

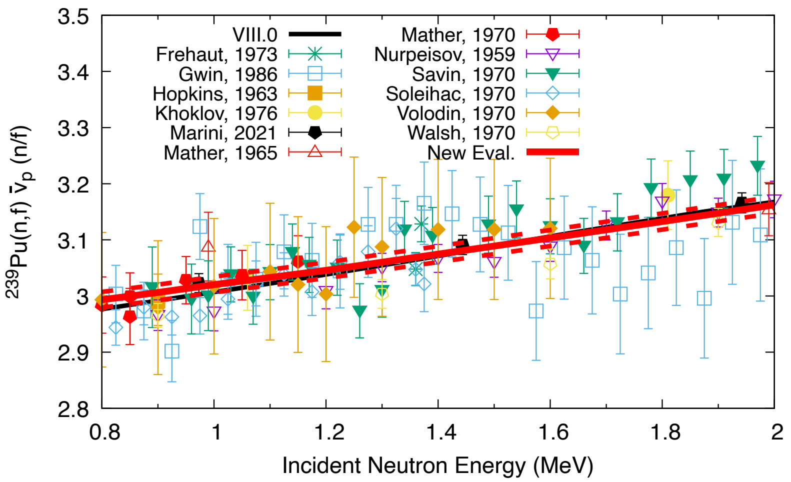
BeoH accurately calculates small yields to the same accuracy as large yields (deterministic).



Chi-Nu data & CGMF evaluation

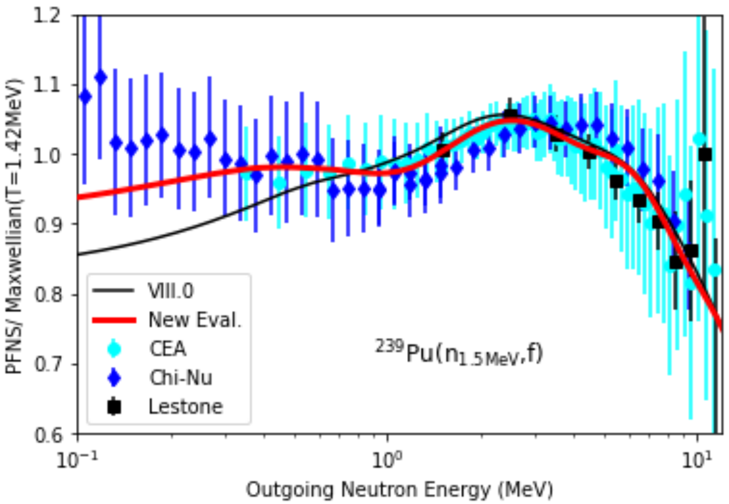
Data Is Used to Improve ^{239}Pu evaluations

Figures: D. Neudecker (LANL/XCP-5)



CGMF modeling has been used to evaluate $\bar{\nu}$ for the first time. PFNS evaluation using the Los Alamos model.

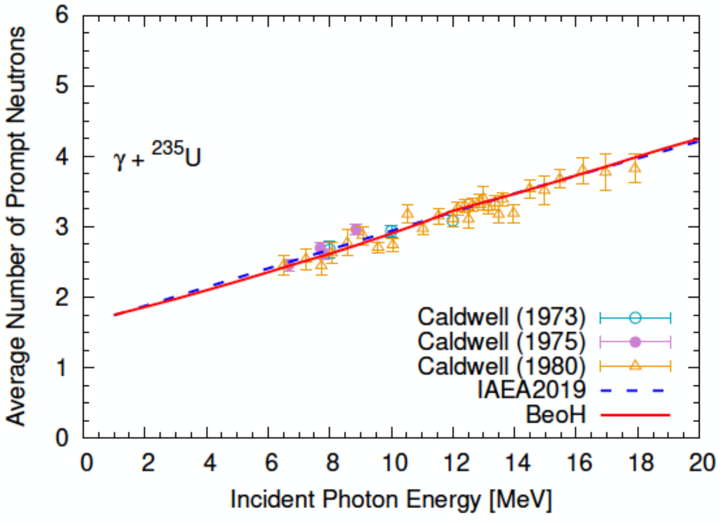
Evaluations performed by D. Neudecker (LANL/XCP-5)

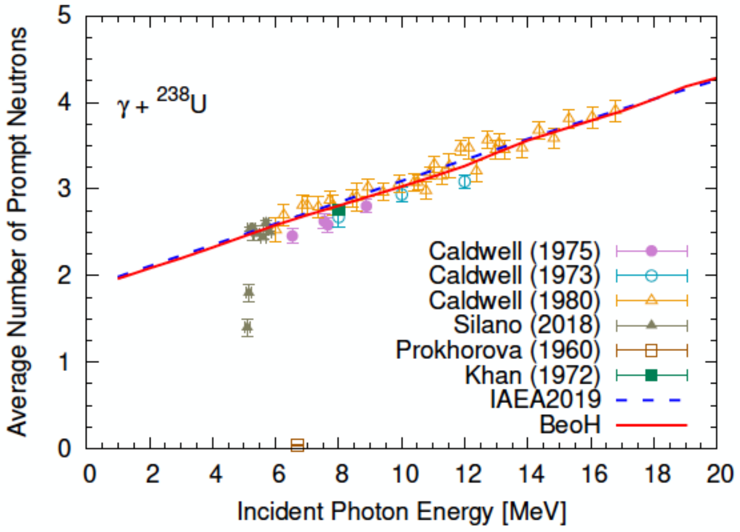


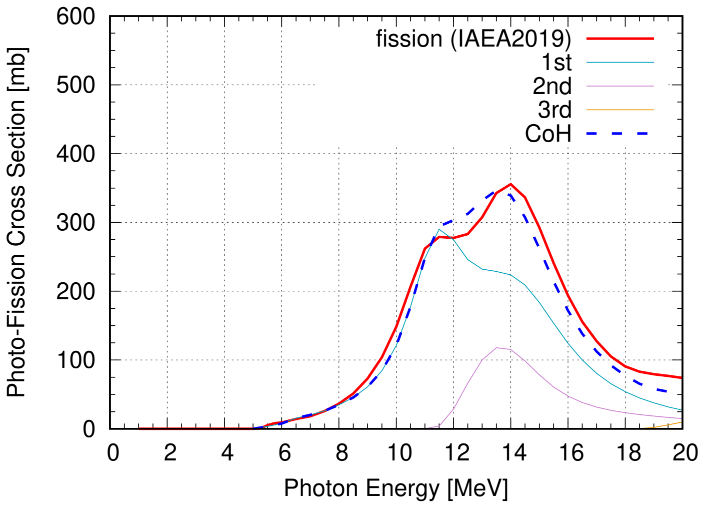
- A CEA collaboration used Chi-Nu to measure very precise $\bar{\nu}$ data which was combined with CGMF modeling for a recent evaluation.
- LANL Chi-Nu PFNS measurements extended the range of incident and outgoing neutron energies for improved evaluations.
- Combined - with an updated (n,f) cross section evaluation – changes to fission observables perform well in critical assembly benchmarks.

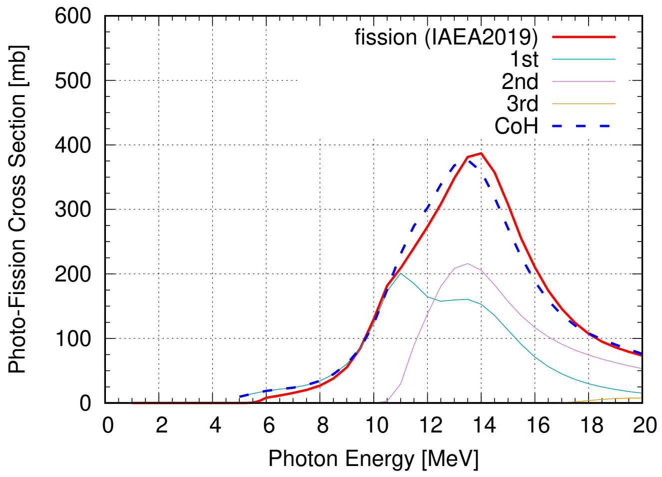
CoH/BeoH Extended to Photon-Induced Multi-Chance Fission

Photo-nuclear reaction on ^{235}U, ^{238}U, and ^{239}Pu calculated based on the BeoH model parameters obtained by Shin Okumura for the neutron-induced fission calculations [JNST **59**, 96 (2022)]

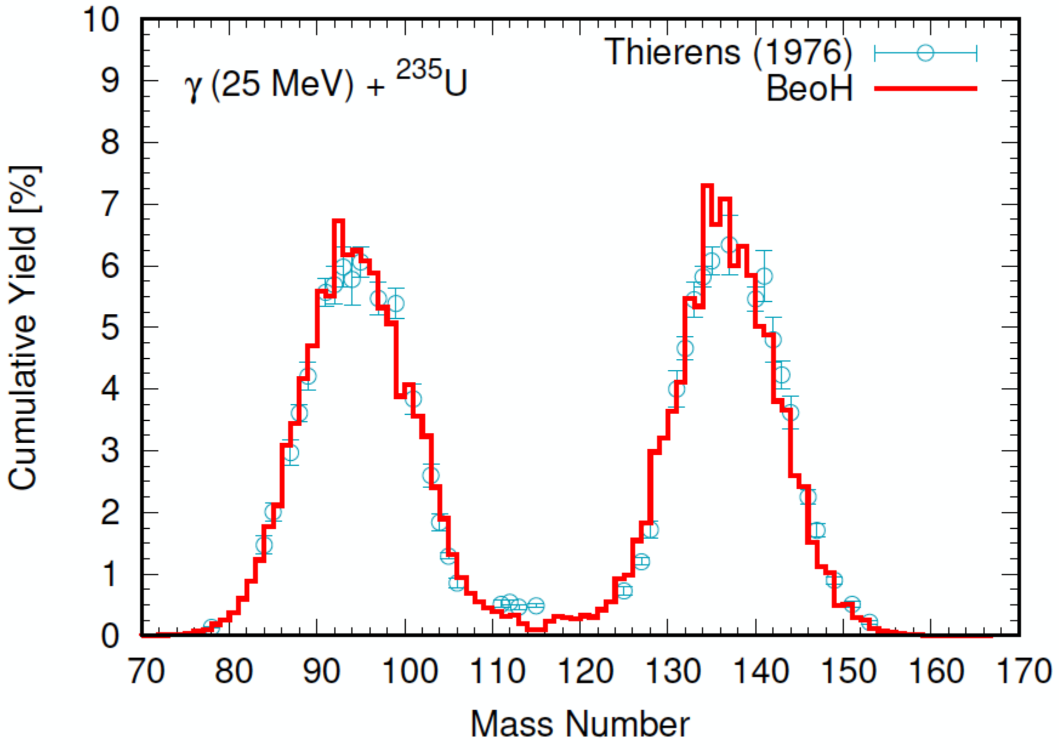


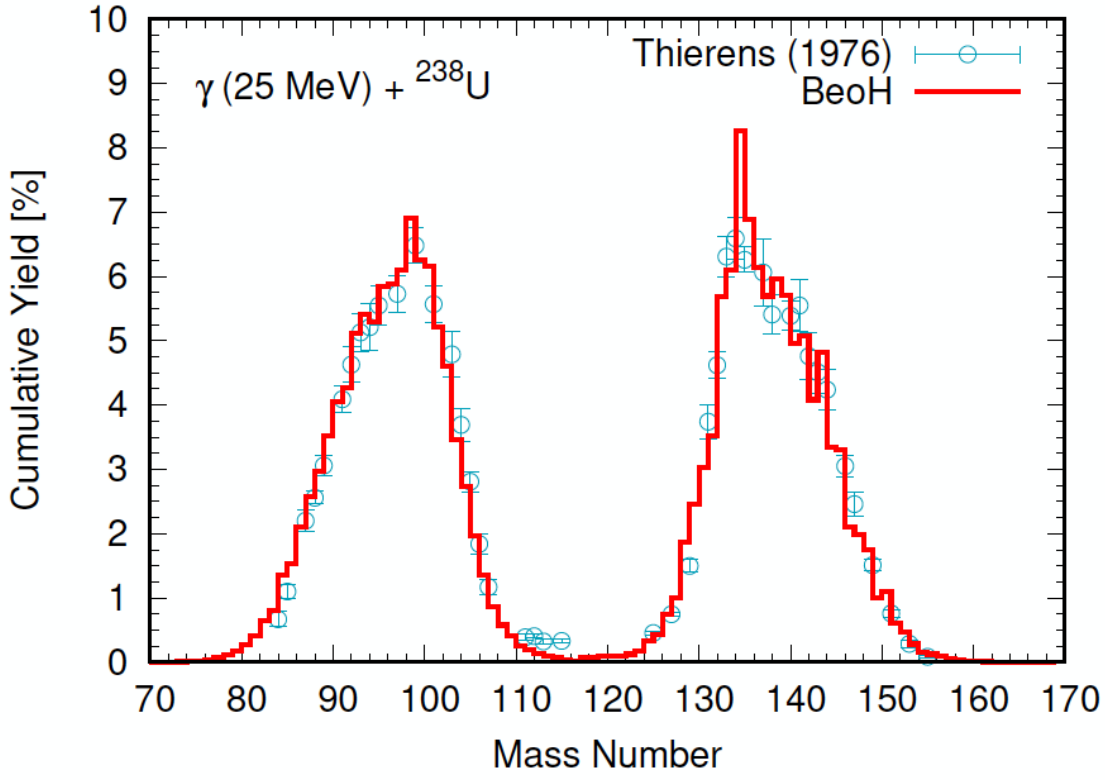






Photofission product yields (preliminary)

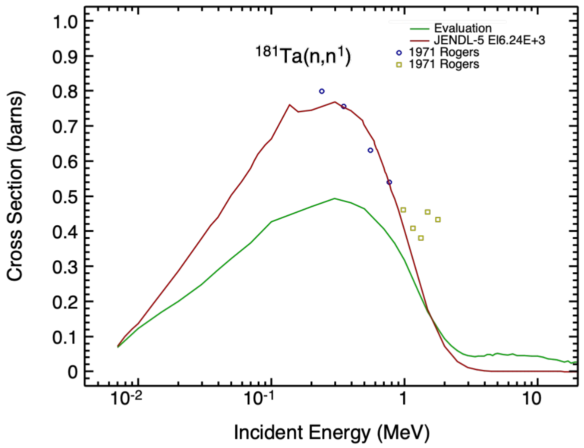


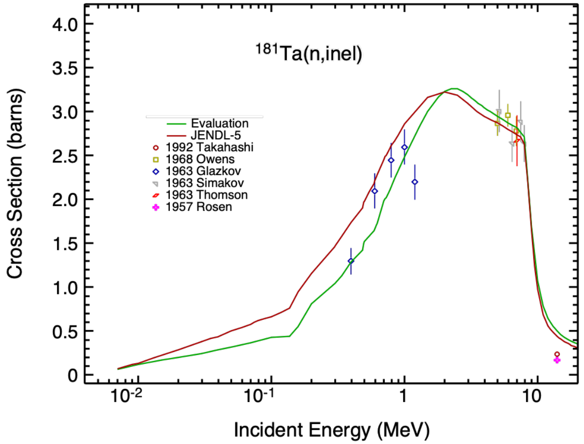


No fit to the data (default parameters)

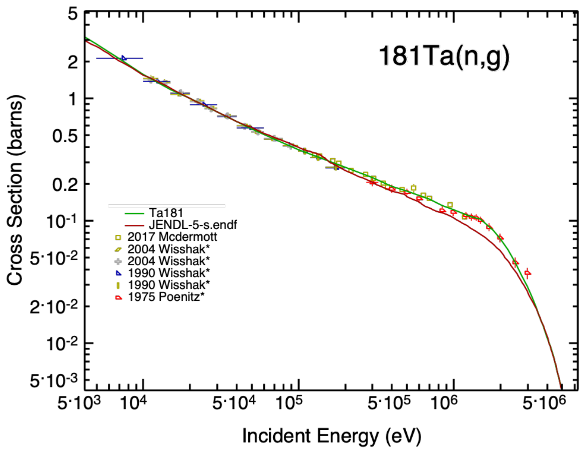
^{181}Ta evaluation

Consistent, model based (EMPIRE) evaluation reproducing selected differential data and well performing in integral testing



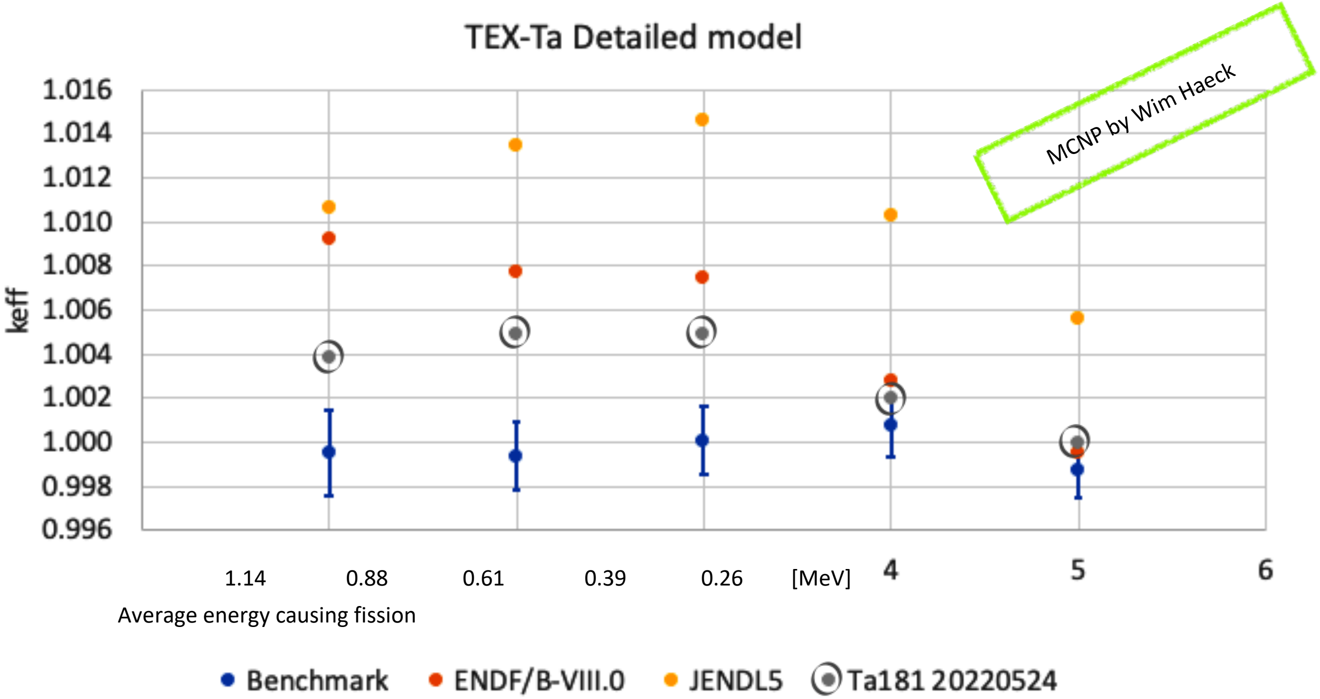


- 1st inelastic - major difference to JENDL5 driven by modeling consistency
- Capture - model forced to follow selected experimental data



Tex (new experiment) - essential improvement compared to ENDF/B-VIII.0 and JENDL-5.0

Further amelioration possible with the new ^{239}Pu



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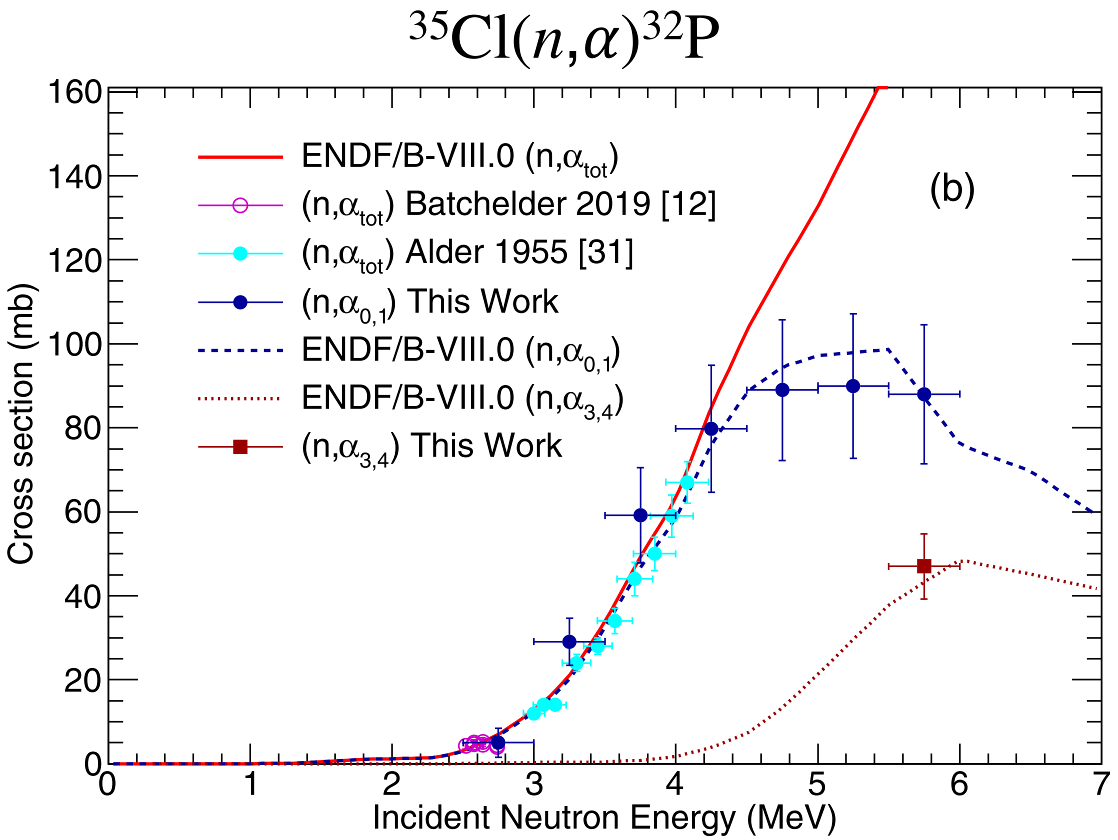
Medium mass evaluations

LANL CoH3 Hauser-Feshbach code

Recent measurements

- Chlorine: ^{35}Cl(n,p)
  - calculation performed for *PRC102, 024623* paper including all the other reaction channels
  - final evaluation planned soon
- Nickel: ^{56,58,59,60}Ni(n,p), (n,d), (n,a)
  - full evaluations 58,59,60 performed in the past
  - new update based on LENZ data underway in collaboration with KAERI
- Iron: ^{54,56}Fe(n,p), (n,d), (n,a)
  - new update based on LENZ data underway in collaboration with KAERI and BNL
- Zinc: ^{64,66}Zn(n,p), (n,d), (n,a)
  - under assessment/developing work-plan



Experimental data from LENZ: summing the yield for the (n,α_0) and (n,α_1) reaction channels, shows good agreement with the current ENDF/B-VIII.0 library.

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Light-element R-matrix evaluation

R-matrix evaluation

Observation
- ***Single*** experiment observations of yield
- Unpolarized: $\sigma_{tot}, \sigma, \sigma(\theta)$
- Polarization: $P_n(E,\theta), A_y(E,\theta), K_x^{x'}, \ldots$

e.g. $\sigma(^{16}\mathrm{O}(n,n)^{16}\mathrm{O})$, $P_n(^{13}C(\alpha,\vec{n})^{16}O)$

Compilation
- Combination of single-experiment ***differential*** data (EXFOR/CSISRS)
- ***Compound-system*** data deck

e.g.: $^{17}\mathscr{O} = {}^{16}\mathrm{O}(n,n_i) + {}^{13}\mathrm{C}(\alpha,\alpha) + {}^{13}\mathrm{C}(\alpha,n_i) + {}^{16}\mathrm{O}(n,\alpha) + \cdots$

RULE: Include ***all*** data

Evaluation
- Determination of initial parameters $(E_\lambda, \gamma_{\lambda,c})$ from known/guessed resonance structure (ENSDF, TUNL-NDEP)
- Optimization of $\chi^2 = \sum_{\mathrm{expt's}} \chi^2_{\mathrm{expt}}$

Reaction Data
- Energy, angle, energy-angle dependent data formatting
- Formats: ENDF-6, GNDS, *etc*.

Structure & Decay Data
- Resonance properties: $E_j, \Gamma_{\mathrm{tot,j}}, \Gamma_{j,c}, C_{j,c}$
- Formats: RIPL, ENSDF, ANR

Recent LANSCE light-element measurements

- LENZ: $^{12}C(n,\alpha_0)$; $^{12}C(n,p_0)$; $^{12}C(n,d_0+p_1)$; $^{13}C(n,\alpha_0)$: $\mathrm{E_n} > 7$ MeV*
- CoGNAC: $^{12}C(n,n'\gamma)$; $^{6}Li(n,n'\gamma)$; $^{7}Li(n,n'\gamma)$*
- LENZ: $^{16}O(n,\alpha)$ *[See next slide]*
- $^{6}Li(d,n)$: LANSCE personnel, measurement @ Notre Dame

**Pending EDA$_{f90}$ upgrade*

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