Los Alamos Updates to nuclear data evaluations

Overview:
- Light element evaluations
- $^{208}$Pb evaluation
- Minor actinide evaluations
- Summary
LANL Light-element (LE) evaluations

- Multichannel, unitary: fit all reaction/scattering data simultaneously
- Fit quantum mechanical amplitudes, not cross sections
- Superior to single-channel & cross-section curve fitting
- High-fidelity, low chi-squared: $\chi^2/DOF \sim 1.2 – 1.5$

Core capabilities/efforts

- LANL lead contributor LE evaluations for ENDF/B-VIII.0 (see table below)
- LE evaluations for many users/formats (ENDF, NJOY, ACE, NDI, etc.)
- Provide covariance information for all LE evaluations
- International efforts (IAEA Consultant’s Meeting R-matrix evaluations/Standards)

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Catalogue of some light-element evaluations

NCSP evaluations of interest

- NN, $^9$Be, $^{12/13}$C, $^{16}$O

EDA Code Modernization

- NCSP FY20 request
- Higher-energies (<20 MeV)
- Interface EDA & NJOY, etc.

Roman numerals refer to ENDF versions

-- All LANL evaluations except *

-- * denote LLNL evaluations
CoH$_3$: Coupled-Channels Hauser-Feshbach code

- Hauser-Feshbach-Moldauer theory for compound nucleus reaction
  - 45,000 lines C++ code (~ 140 C++ source files, ~60 headers, ~80 classes)
  - maintain by GNU Autotools package

- Modules and Models employed
  - spherical and deformed optical models
  - DWBA for direct inelastic scattering
  - Moldauer’s width fluctuation correction with LANL parametrization
  - Gilbert-Cameron level density with updated parameters
  - pre-equilibrium 2-component exciton model
  - Madland-Nix prompt fission neutron spectrum including pre-fission emission
  - direct/semidirect capture model
  - mean-field models (FRDM and Hartree-Fock BCS)

Consistent evaluations in all channels
CoH₃ New Evaluation of $^{208}$Pb, (n,n’), (n,2n), and (n,3n)

Pre-equilibrium estimated by the single-particle model based on FRDM

Strutinsky shell correction predicts lower single-particle level density
- lowers the pre-equilibrium emission
- increase (n,2n)

New evaluation better agrees Simakov data

Need to re-investigate if Frehaut data should be renormalized
CoH₃ New Evaluation of $^{208}$Pb, Capture and Elastic

Very small capture cross section
Realistic Direct/Semidirect capture theory applied (evaluations are simple Lorentzians)

Unphysical dips near 60 and 140 degrees removed
Evaluation similar to JENDL-4
Evaluation of $^{234,236}$U

- **Extensive and consistent** evaluations based on CoH3 calculations, with parameters adjusted to experimental data (DANCE, WNR)
- All open channels included
- KALMAN-based evaluation for fission channel to include cross section data from WNR
- $^{234}$U: re-evaluation of nubar, consistent PFNS
- $^{236}$U: re-evaluation of nubar above 2$^{\text{nd}}$ chance fission, PFNS
- PFGS and gamma multiplicity taken from the recent $^{235}$U evaluation
Evaluation $^{234,236}$U (capture)

- Resonance parameters for $^{236}$U(n,γ) refitted to DANCE data, but only for the s wave and in different format than currently in ENDF (new fit this summer?)
- Data for $^{234}$U(n,γ) will be analyzed this summer (before September?)
- CoH$_3$ evaluation
  - Width corrections fluctuation of Moldauer, with the Engelbrecht-Weidenmüller transformation (strict treatment of the directly coupled channels in the Hauser–Feshbach theory), the coupled-channels optical potential of Soukhovitskii
  - Same parameters used for the suite of U isotopes

Baramsai et al, PRC 96 (2017) 024619
$^{234}$U evaluation: all channels consistent from CoH$_3$ calculations
New paradigm for nuclear data evaluations

• **Novelty in evaluation procedure:**
  • Include >1000 integral experiments of various types
  • Develop infrastructure for re-adjustment of existing evaluations each time any evaluation is changed

• **Prerequisites**
  • Reliable set of integral experiments (with input decks)
  • Library of inputs and scripted procedures allowing for quick re-evaluation
  • ML techniques for tracing outliers (in experiments and evaluations), for performing global adjustment and analysis of the results
  • Reaction modeling adequate to reproduce experimental data (all reaction mechanisms)
  • Extensive set of sensitivities
  • Automated validation
  • Integration of experimental, evaluation and validation communities

• **Benefits**
  • Accounting for differential and integral exp. on the same footing
  • Extensive set of covariances including cross-material correlations
  • Reduction of error compensation
  • Improved responsiveness to new measurements and model advances
Summary

- Extend light-element evaluations: higher energy via code modernization
- Improved evaluation for $^{208}$Pb
- Complete and consistent evaluations for $^{234,236}$U
- CoH3: extensive (many models) and flexible evaluation tool neutron induced reactions on medium and heavy nuclei
- New evaluation scheme using ML algorithms

Work in progress:
- Identify benchmarks that include $^{234}$U/$^{236}$U and check the performance of the evaluation
- Include the s-wave parameters for $^{236}$U(n,γ) (DANCE)
- Compare with $^{234}$U(n,γ) cross section, when the analysis is finished
- Neudecker: updates of PFNS for U and Pu based on new ChiNu data
- Kawano, Stetcu, Talou: new deterministic Hauser-Feschbach cascade model for PFNS/PFGS
- Adjustments to CGMF parameters so it can be used in future evaluations