Evaluation work @ LANL for ENDF/B-VIII relevant to the NCSP

Nuclear Criticality Safety Program
Annual Technical Program Review
14-15 March 2017
Washington, D.C.

M. Paris, G. Hale, A. Kahler, T. Kawano, I. Stetcu, P. Talou
Group T-2
Los Alamos National Laboratory

14 March 2017

Los Alamos NATIONAL LABORATORY EST.1943

NNSA National Nuclear Security Administration
Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Overview: LANL/T-Div. nuclear data evaluation project

- **Organizing principle**
  - Comprehensive, consistent theoretical modeling
    - Constrain nuclear data evaluations
    - Consistent with the quantum theory (when possible)
    - Quantify uncertainty
- **Synergistic efforts**
  - NNDC: ENDF/B-VIII.β4 tagged 2017 Feb 28
    - ***NB: criticality has been affected***
    - Dave Brown tomorrow morning
    - drafting *Nuclear Data Sheets* manuscript (to appear 2018 January)
  - CIELO collaboration (NEA WPEC-Subgroup 40)
    - https://www-nds.iaea.org/CIELO/
  - IAEA Standards
  - Array of end-point users
    - Nuclear security, energy, basic research

- **Exp't collaborations**
  - DANCE and JRC (Geel) for prompt fission gamma-ray spectra
  - Chi-Nu & RPI for prompt fission neutrons
  - LENZ for *e.g.* $^{16}O(n,\alpha)$

Outline

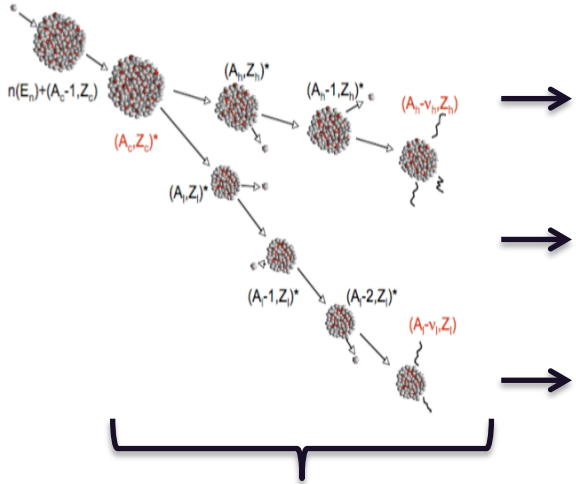
- **Heavy/fission analyses**
  - Codes overview/development
    - CoH; DeCE; CGMF; NJOY2016/21
  - Evaluation work:
    - Prompt fission neutron spectra
    - Prompt fission gamma-ray evaluations
    - Updated cross sections for ^{59}Co
    - New elastic scattering angular dist's ^{208}Pb

- **Light element analyses**
  - R-matrix analyses: EDA code
  - ENDF/B-VIII.0 ^{16}O evaluation
    - Low-energy scattering cross sections
    - ^{13}C(α,n) and ^{16}O(n,α_0) cross sections
    - Fits, data renormalizations, etc.
    - Differences with VII.1
    - Data testing; β4 released
  - ENDF/B-VIII.0
    - ^{12,13}C evaluations
    - Light-element standards
      - ^{1}H, ^{6}Li, ^{10}B, and C
  - Modern/modular code development
    - EDA6 (Fortran2003 version of current EDA5/F77)
    - ENDF-6/GND interface

Heavy system analyses

Monte Carlo Hauser-Feshbach (CGMF)

- Hauser-Feshbach statistical theory of nuclear reactions
  - Neutron and γ-ray emission probabilities calculated and sampled at each stage of the decay
- **CGMF**: Monte Carlo implementation
- Full kinematic reconstruction of fission fragments, neutrons and gammas emitted



Prompt emissions of n and γ within 10^{-14} sec

→ Monte Carlo histories of fission events

$$A, Z, KE, U_i, J_i, \pi_i, \nu_n, \nu_\gamma$$
$$\vec{p}_F(\text{pre}), \vec{p}_F(\text{post}) \text{ in LAB frame}$$
$$\{\vec{v}_{n_i}, E_{n_i}\}_{i=1,\nu_n}, \{\vec{v}_{\gamma_j}, E_{\gamma_j}\}_{j=1,\nu_\gamma}$$

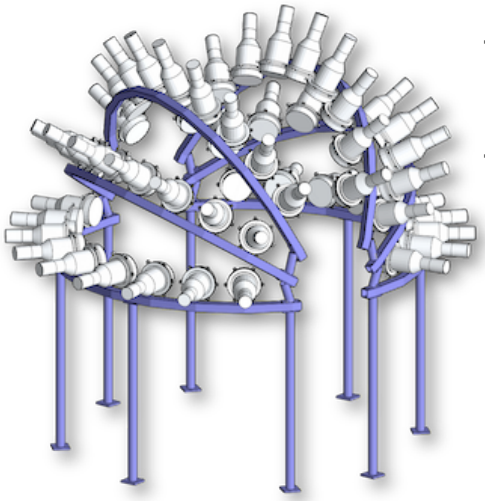
Recent code development

- **CoH**
  - Inclusion of M1 “scissors” mode in strength function
    - strongly impacts abs norm of capture cross section [PRC 89, 034603, 2014]
- **DeCE**
  - ENDF formatting tool; open source https://github.com/toshihikokawano/DeCE
- **CGMF**
  - Extending actinide analyses
    - fission fragment mass and charge yields [from Moller (LANL T-2)]
  - **Global and consistent** evaluations of prompt neutrons and gamma rays
    - Various studies in progress
  - Synergistic effort with NA22 to implement CGMF into MCNP6.2 release
    - Current effort to improve precision of criticality predictions
  - NJOY2016 open source release [Skip Kahler* (LANL T-2) tomorrow 11:25a]
    - Development of NJOY21 is in progress [Jeremy Conlin LANL XCP-5]

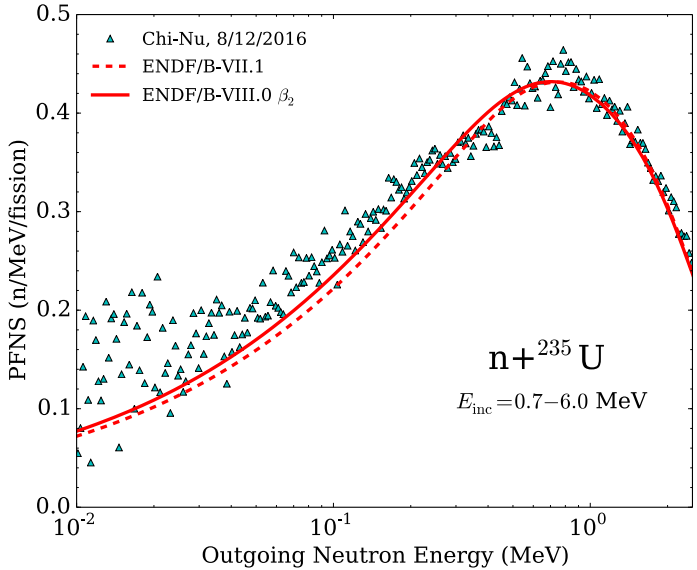
*Last TPR

Prompt fission neutron spectra evaluations

- **X_v (Chi-nu) @ LANSCE**
  - ^{235}U: low-energy array
  - ^{239}Pu awaiting data
- **Prompt fiss. n mult. dist. P(v)**
  - CGMF+Terrell < 20 MeV U8/9/P9
  - Proposed new ENDF-6 format
    - CSEWG accepted
  - P(v,E_{inc}) inclusion in B-VIII.0



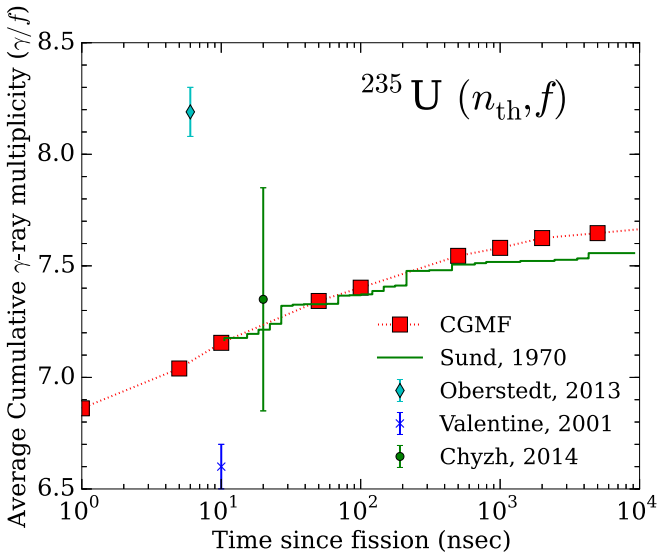
Chi-nu high-energy detector with high- & low-energy arrays

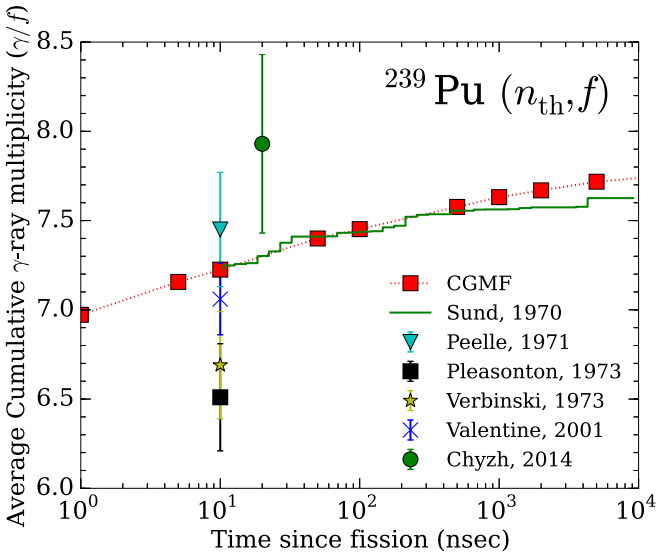


- **New evaluations U5/P9**
  - Model: CoH+Madland-Nix
  - Improved high-energy models
    - Multi-chance fission; pre-eq; corrected (n,xnf) spectra
  - ENDF-6 format for B-VIII.0 rls.

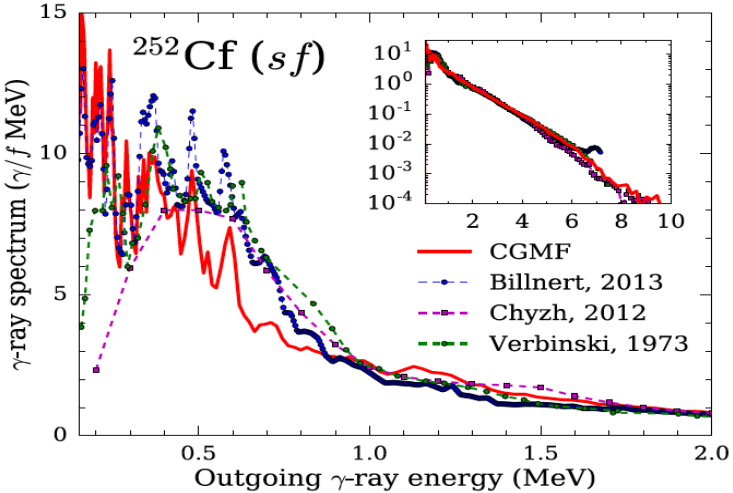
Prompt fission gamma-ray evaluations

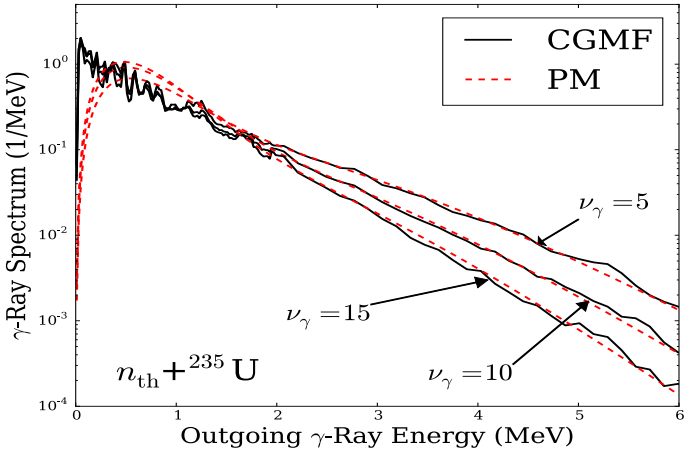
- **Calculations performed using CGMF**
  - Gamma-multiplicity dependent spectra calculated for the first time
    - very good agreement with experimental data from DANCE (LANSCE)
  - New evaluated files prepared for ENDF/B-VIII.0 (in testing)
  - Time-dependent gamma multiplicity (*PRC 94, 064613, 2016*)



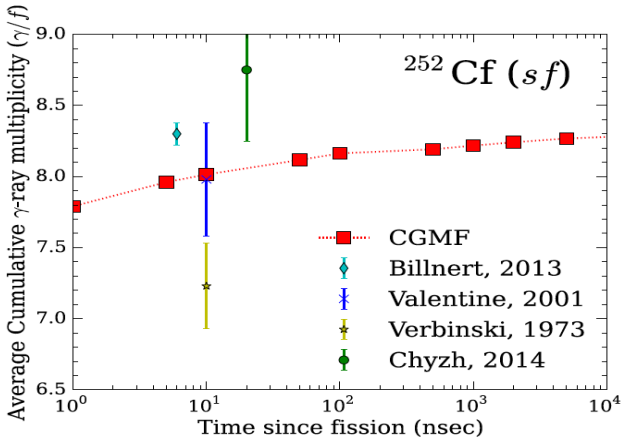


Prompt fission gamma properties



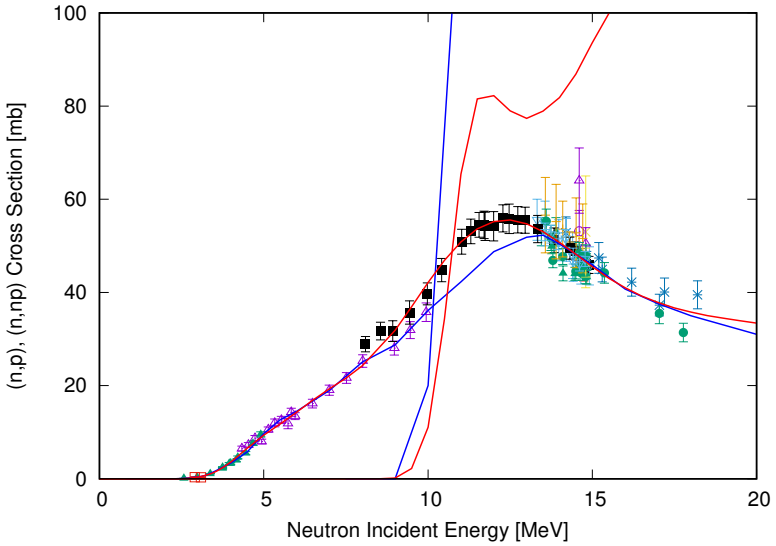


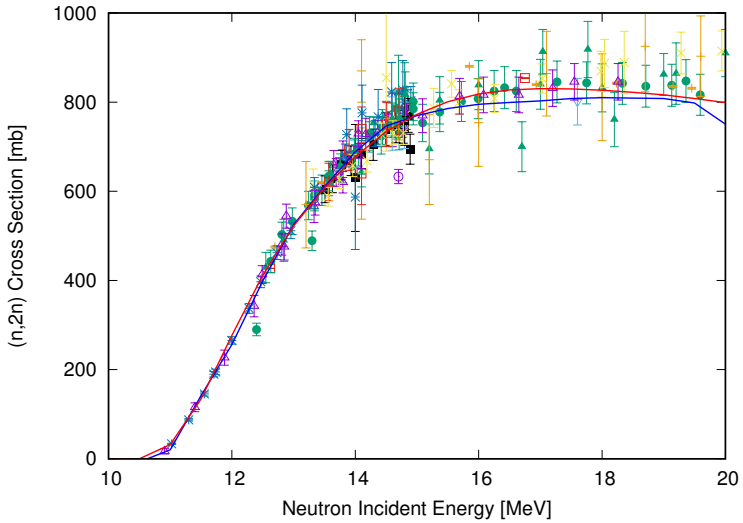
- Simulations reproduces features of experiment (discrete transitions in fission fragments). Details depend on the less known nuclear structure information
- Significant dependence of the multiplicity-dependent prompt fission gamma-spectra with multiplicity. Simulations reproduce well the experiment
- Average gamma-ray multiplicity changes significantly with the time coincidence window
- Detailed simulations available for ^{235}U(n,f), ^{238}U(n,f), ^{239}Pu(n,f), ^{240}Pu(sf), ^{241}Pu(n,f), ^{242}Pu(sf).



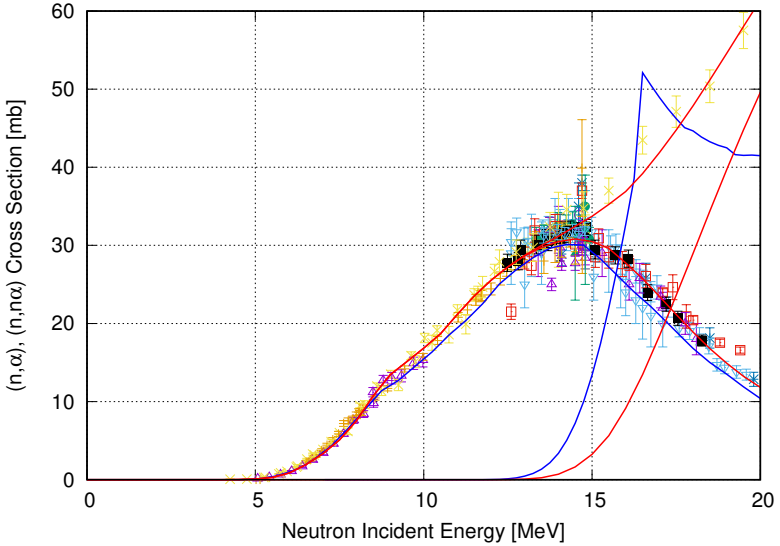
^{59}Co evaluation

- Re-evaluation above 100 keV with CoH_3
- Coupled-channels DWBA calculation
- Updated σ, eng & ang distributions:
  - (n,n'), (n,2n), (n,3n), (n,p), (n,np), (n,α), (n,nα), (n,d), (n,nd), (n,t), (n,3He), (n,2p), (n,pα), (n2np) & (n,γ) (cross-section only)





- ENDF/B-VII.1
- CoH_3



The light stuff

R-Matrix theory ensures analyses consistent with the quantum theory

- Causality (complex analyticity)
- Probability conservation (unitarity)
- Time reversal invariance (reciprocity)

Physical Principle (mathematical req.)

EDA: R-Matrix code features

- Observes above mathematical requirements
- Any spins, masses, charges two-body channels
- Relativistic kinematics and R-matrix parametrization
- All polarization observables for 2➔2 processes
- Fairly general data-handling capabilities (< SAMMY)
- Optimization via variable-metric algorithm
  - ✓ parameter covariances at solution

Recent EDA code development

- **Data handling**
  - Python codes under development
    - XML container “GND”
- **Analysis code**
  - Existing EDA5 (F77) ➔ EDA6 (Fortran2003/2008)
  - Modular/OOP code design
  - EDA6 superset of existing EDA5 features/capabilities
- **Exchange formats**
  - Built-in ENDF-6/GND/ACE(cont.)/NDI(multigroup)/…
- **Uncertainty quantification**
  - Importance function; Bayesian
- **Long(er)-term development**
  - Implementation into integral benchmark codes
    - Concurrent optimization of light and heavy analyses

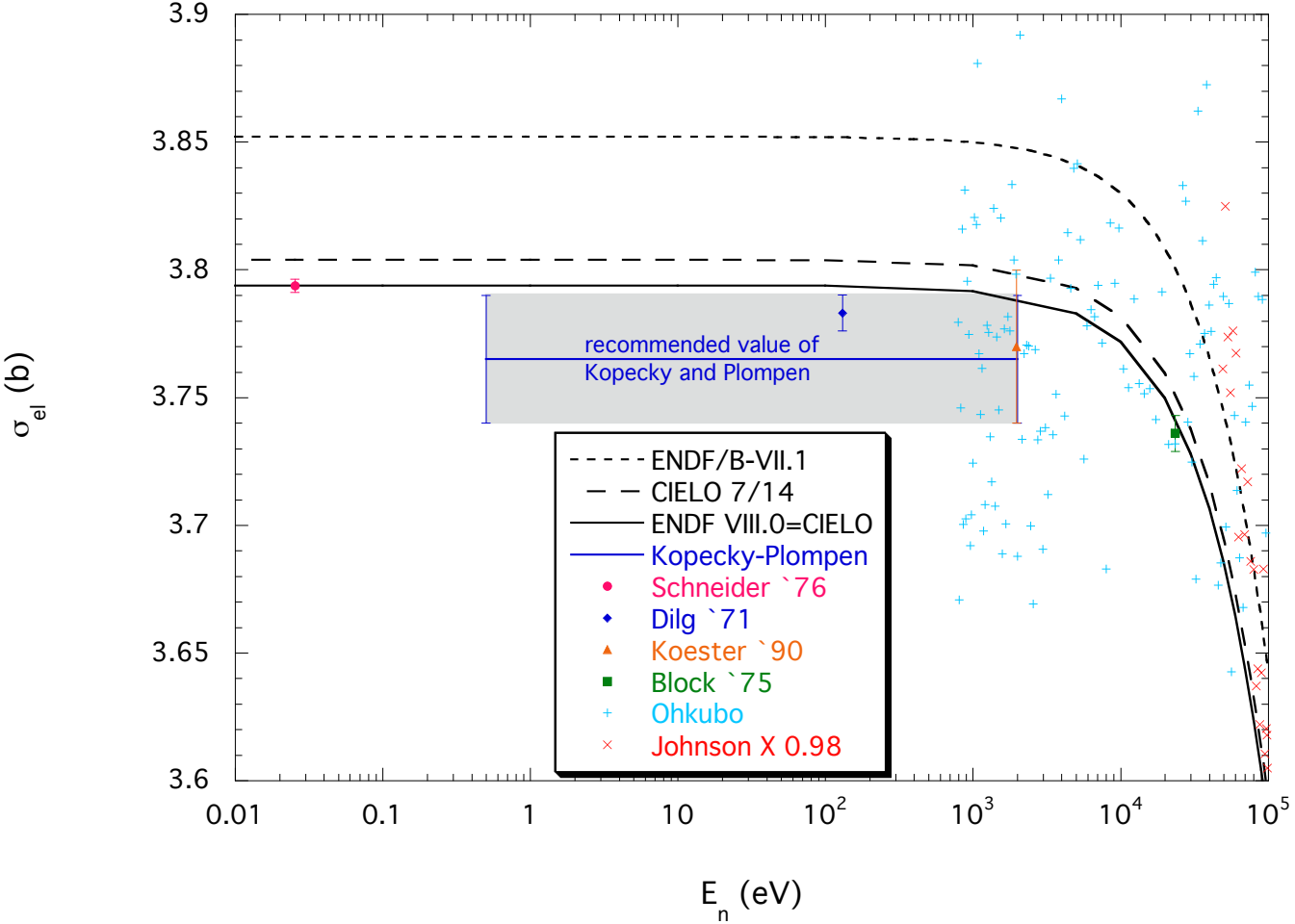
R-Matrix Analysis of Reactions in the ^{17}O System

channel	a_c (fm)	I_{max}
n+^{16}O	4.4	4
α+^{13}C	5.4	5

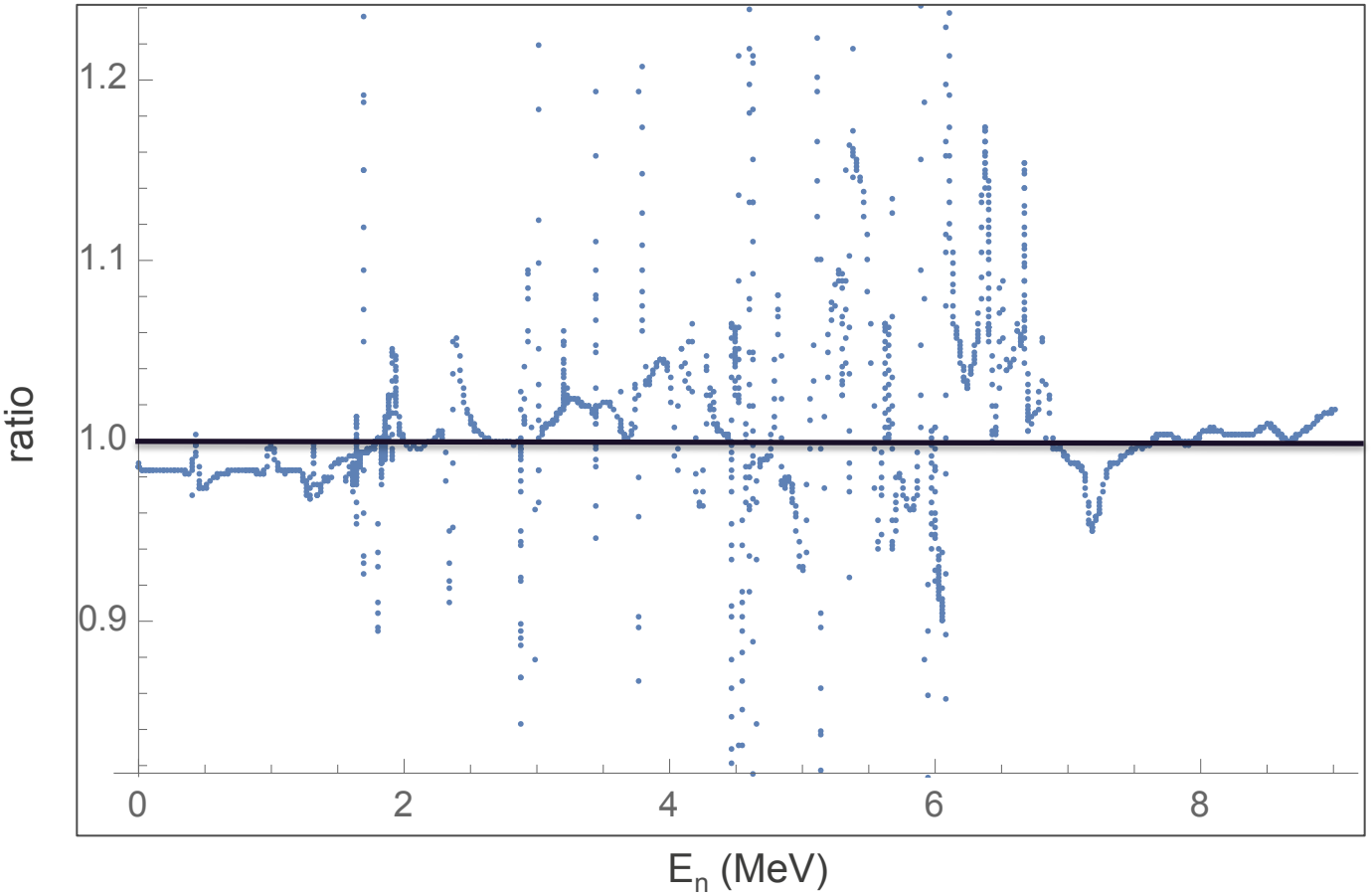
Reaction	Energies (MeV)	# data points	Data types
$^{16}O(n,n)^{16}O$	E_n = 0 – 7	2540	σ_T, $\sigma(\theta)$, $P_n(\theta)$
$^{16}O(n,\alpha)^{13}C$	E_n = 2.35 – 5	672	σ_{int}, $\sigma(\theta)$, $A_n(\theta)$
$^{13}C(\alpha,n)^{16}O$	E_α = 0 – 5.4	870	σ_{int}
$^{13}C(\alpha,\alpha)^{13}C$	E_α = 2 – 5.7	1168	$\sigma(\theta)$
total		5250	8

χ^2 per degree of freedom = 1.68

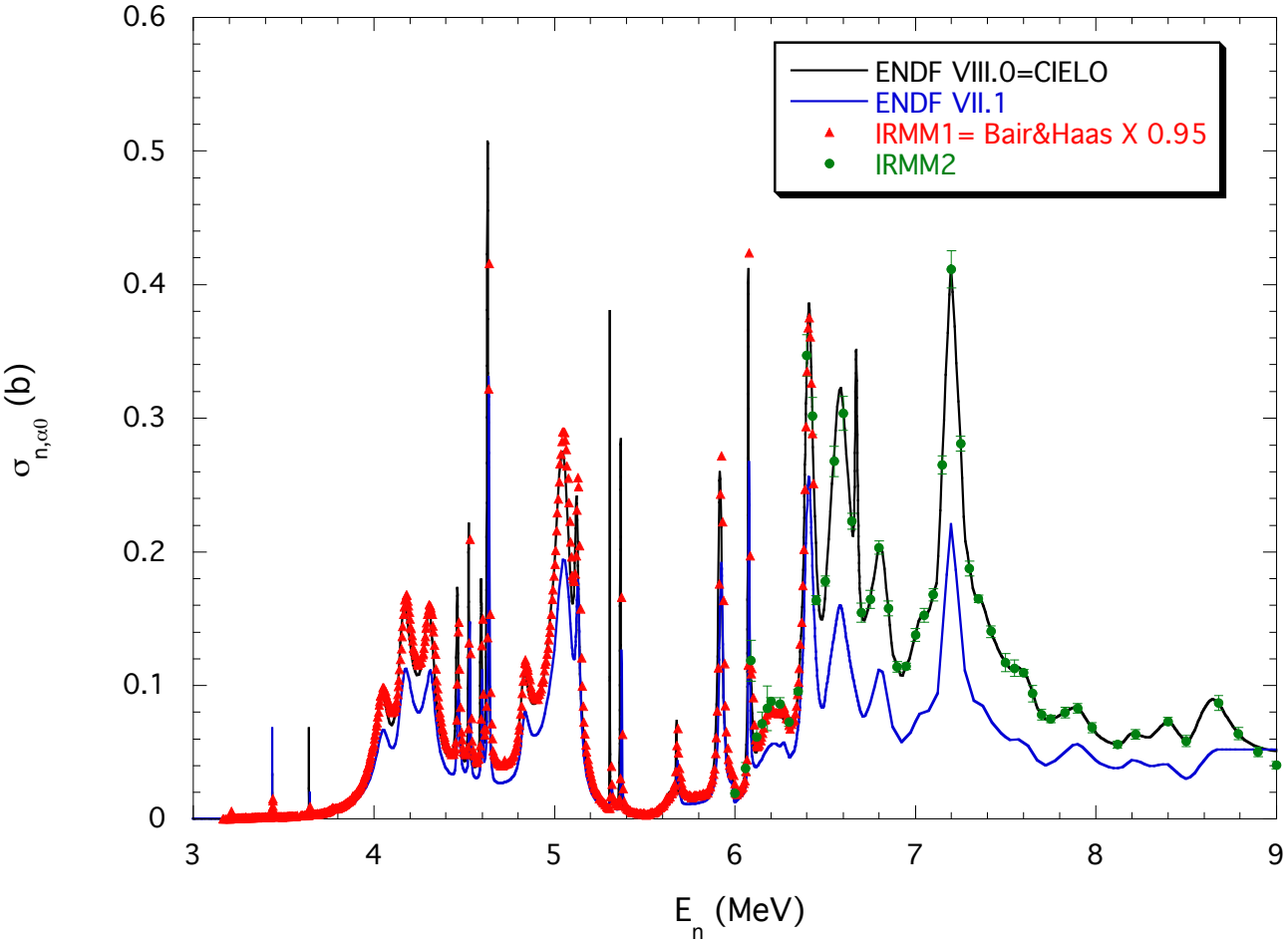
n+^{16}O Elastic Scattering Cross Section



Ratio of ENDF/B-VIII.0/VII.1 σ_T for Oxygen



$^{16}O(n,\alpha_0)^{13}C$ Cross Section

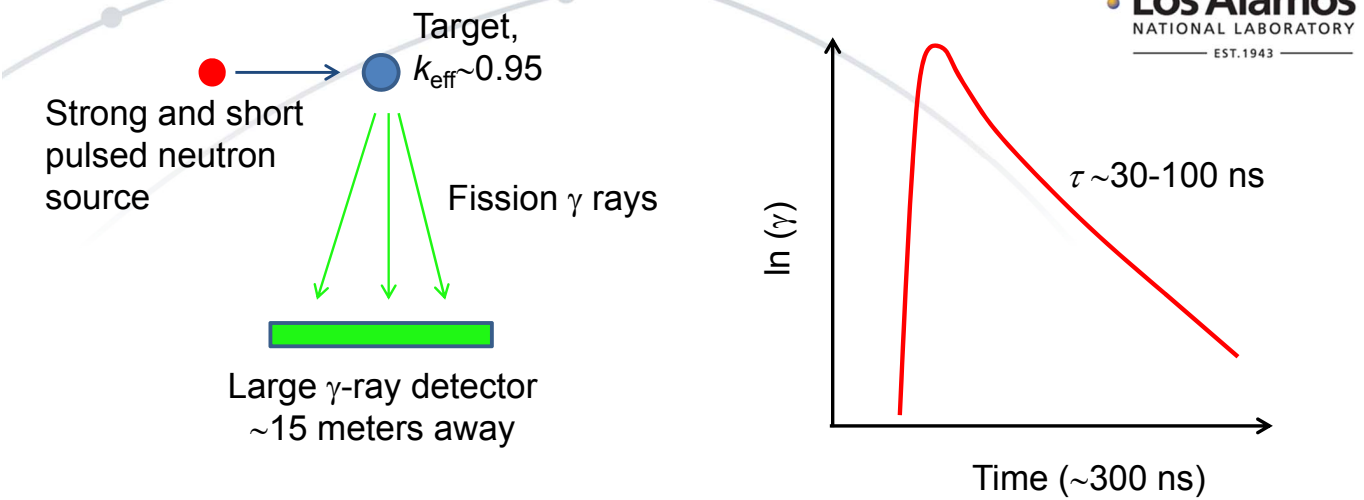


Summary & Outlook

- **Continued advancement in the application of fundamental quantum-theoretical methods to understanding data**
- **ENDF/B-VIII.B4**
- **Improved physical models PFNS & PFGS**
  - CGMF: Multi-chance fission; pre-eq; corrected (n,xnf) spectra
  - CoH: Scissors M1 mode – capture normalization
- **Light element evaluations**
  - Modernization of EDA and auxiliary codes
  - Spectra; many-body final states; *ab initio* calculations
- **Development of integrated codes**
  - Move toward concurrent differential/integral optimization

Thank you

Neutron Diagnosed Sub-critical Experiments (NDSE)



LANL recently funded a LDRD project to measure the time dependence of gamma emission from sub-critical static objects following the irradiation from a strong and short burst of neutrons.

Other fission data of interest to this (and related) projects are :

- The number and time scale of beta-delayed fission.
- The number and energy spectra of γ–rays emitted from fragments on the relevant time scales.
- Fission n and γ–ray multiplicity distributions, correlations between fission n and γ multiplicity and the corresponding energy spectra (for detailed noise analysis).

ENDF/B-VIII.β4 changes

- **Last beta release in which criticality can be affected**
- **Change log highlights**
  - New ^{1}H, ^{56}Fe, ^{235}U, ^{238}U, and ^{239}Pu CIELO evaluations
  - New evaluations incorporating the 2017 Neutron Standards evaluations
    - 6Li, 10B, 197Au
  - New Thermal Scattering Law evaluations from NCSU
    - UN (tsl-UinUN.endf and tsl-NinUN.endf)
  - Many many bug fixes and other improvements
  - Full change log: https://ndclx4.bnl.gov/gf/project/endf/

Status of Prompt Fission γ-Ray Evaluations

- ENDF sections:
  - MF1, MT458: components of energy released in fission
  - MF15, MT18: prompt fission γ-ray spectrum
- ENDF/B-VII.1:
  - U-235:
    - Taken from B-VI
    - Stewart, Alter, Hunter, ENDF-201 (1976) evaluation based on Verbinski and experimental data (100 nsec after fission)
    - Stewart and Hunter, LA-4918 (1972)
  - Pu-239:
    - Taken from B-V.2
    - Hunter and Stewart, LA-4901 (1972)
    - Verbinski et al. data

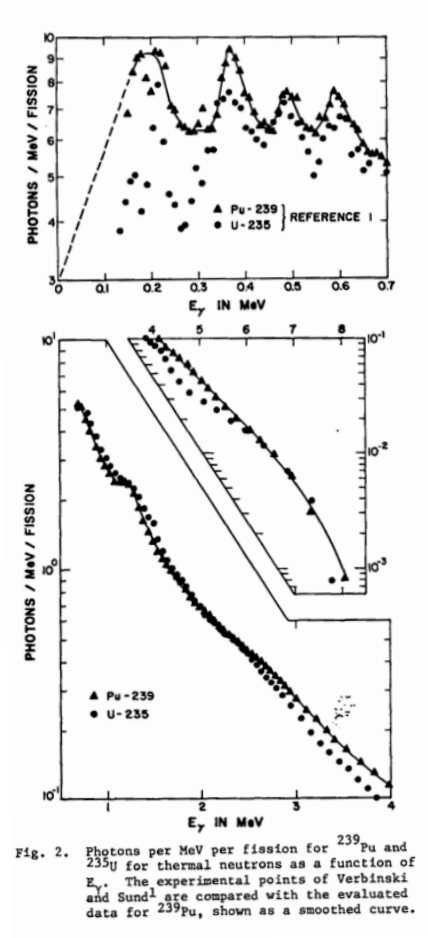
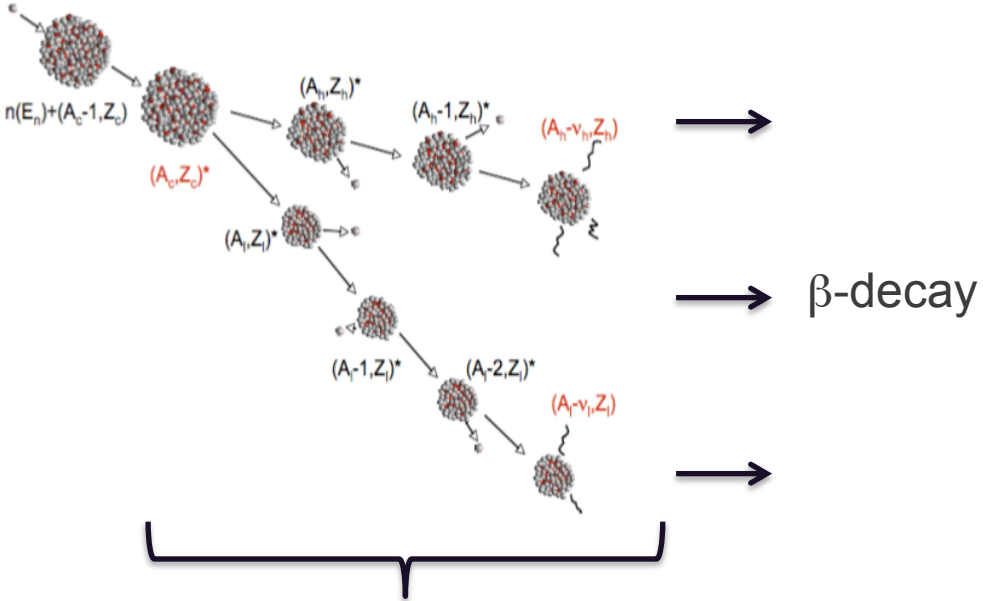


Fig. 2. Photons per MeV per fission for ^{239}Pu and ^{235}U for thermal neutrons as a function of E_γ. The experimental points of Verbinski and Sund[1] are compared with the evaluated data for ^{239}Pu, shown as a smoothed curve.

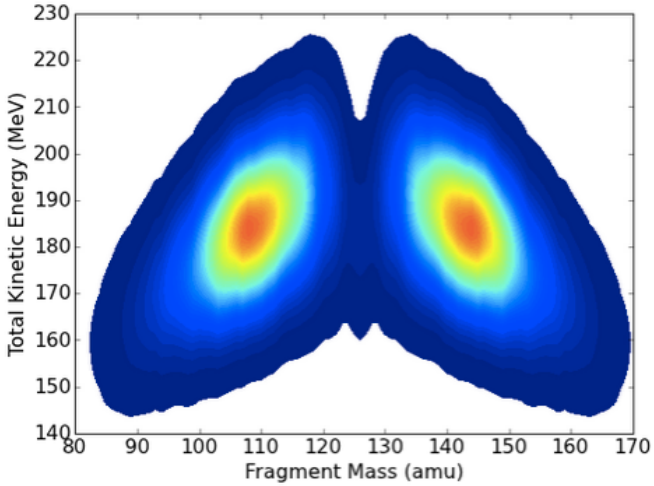
Verbinski, Phys. Rev. C 7, 1173 (1973)

Modeling Prompt Fission Neutrons/Gamma Rays (CGMF)



β-decay

Prompt emissions of n and γ within 10^{-14} sec

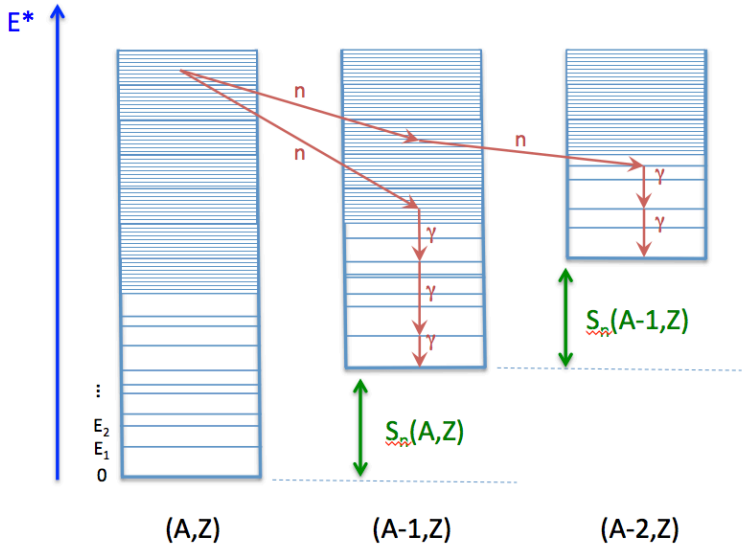


Fragment Yields Y(A,TKE) in ^{252}Cf (sf)

Goal: follow the sequential emissions of prompt neutrons and γ rays from the excited primary fission fragments, event-by-event.

Monte Carlo Hauser-Feshbach (CGMF)

- Hauser-Feshbach statistical theory of nuclear reactions
  - Neutron and γ-ray emission probabilities calculated and sampled at each stage of the decay
- **CGMF**: Monte Carlo implementation
- Full kinematic reconstruction of fission fragments, neutrons and gammas emitted



→ Monte Carlo histories of fission events

$$A, Z, KE, U_i, J_i, \pi_i, \nu_n, \nu_\gamma$$
$$\vec{p}_F(\text{pre}), \vec{p}_F(\text{post}) \text{ in LAB frame}$$
$$\{\vec{v}_{n_i}, E_{n_i}\}_{i=1,\nu_n}, \{\vec{v}_{\gamma_j}, E_{\gamma_j}\}_{j=1,\nu_\gamma}$$

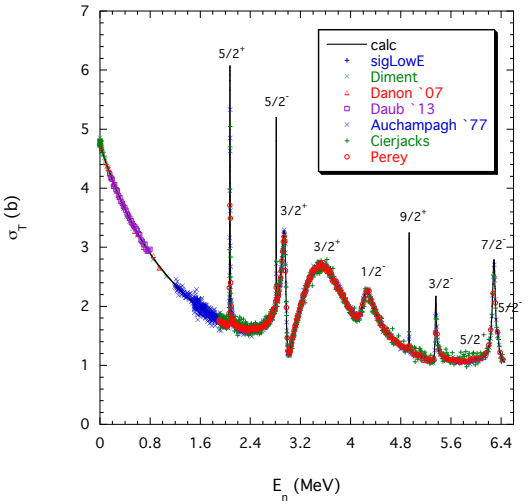
Analysis of Reactions in the ^{13}C System

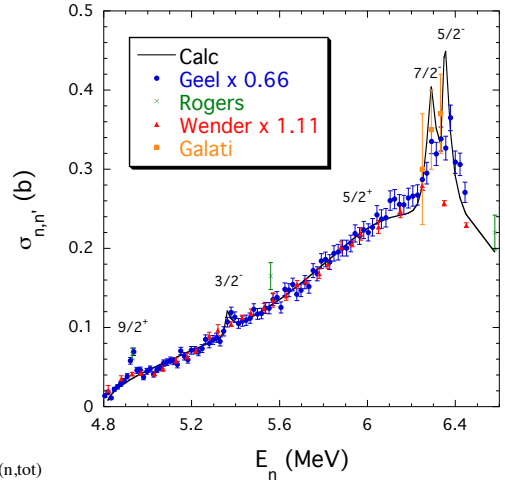
channel	a_c (fm)	l_{max}
$n+^{12}C(0^+)$	4.6	4
$n+^{12}C^*(2^+)$	5.0	1
$\gamma+^{13}C$	50	1

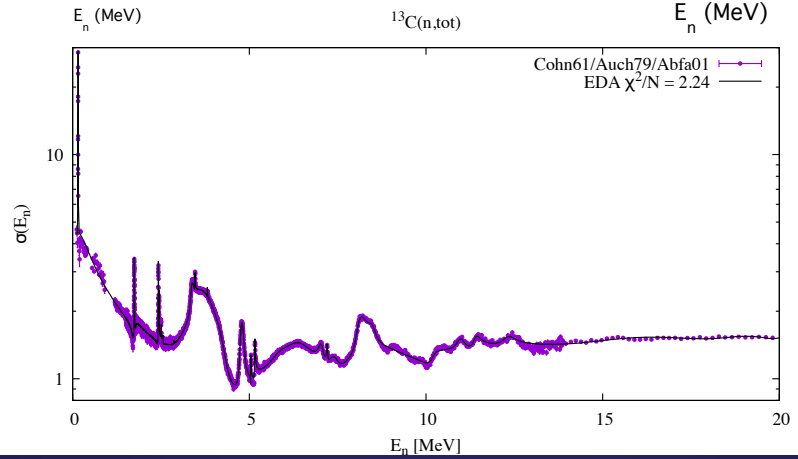
Reaction	Energies (MeV)	# data points	Data types
$^{12}C(n,n)^{12}C$	$E_n = 0 – 6.45$	6940	σ_T, $\sigma(\theta)$, $A_n(\theta)$
$^{12}C(n,n')^{12}C^*$	$E_n = 5.3 – 6.45$	443	σ_{int}, $\sigma(\theta)$
$^{12}C(n,\gamma)^{13}C$	$E_n = 0 – 0.199$	7	σ_{int}
total	4994	7390	5

χ^2 per degree of freedom = 1.54

n+^{12,13}C Cross Sections

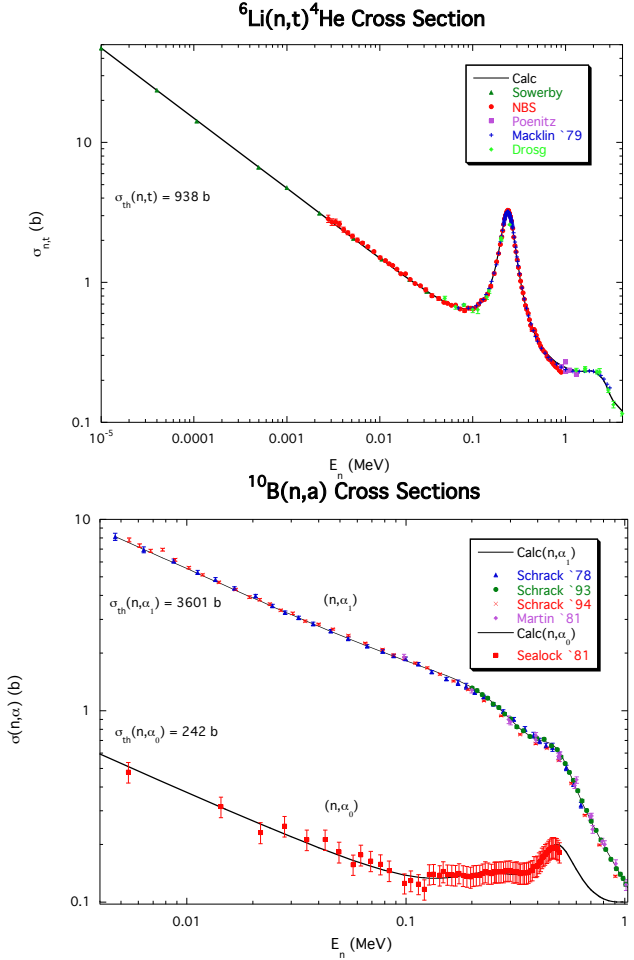




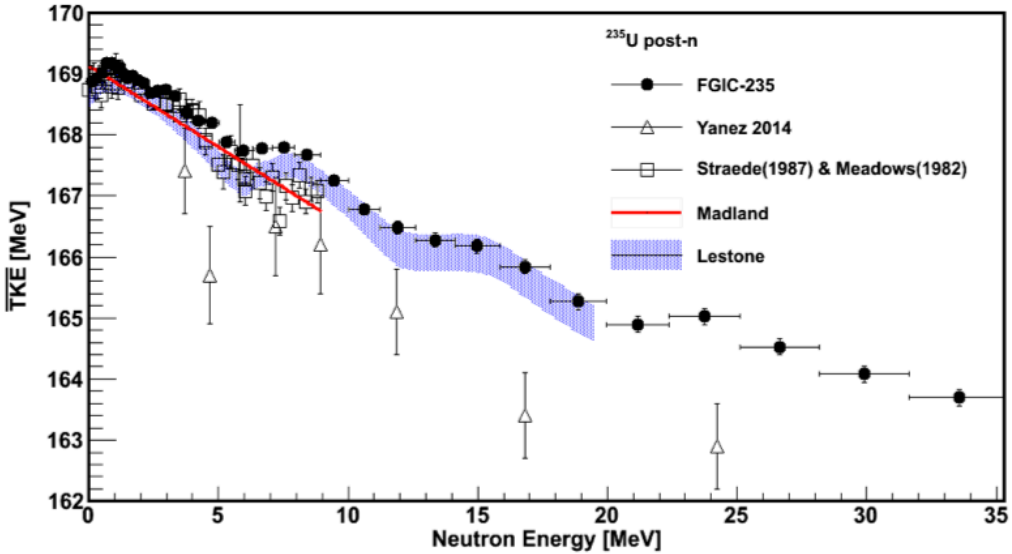


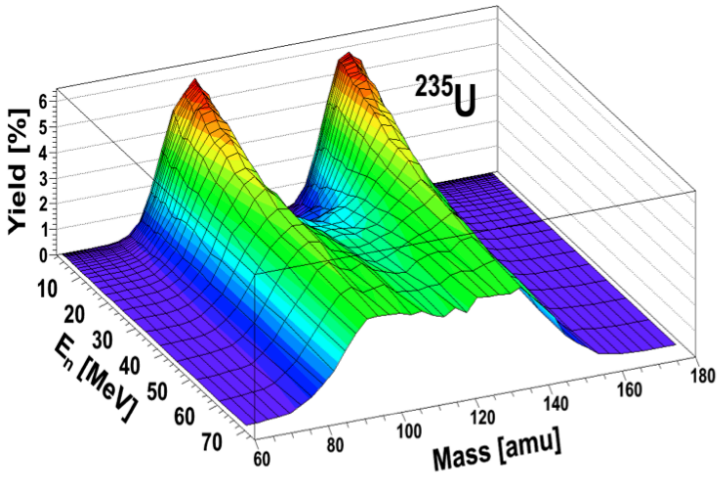
Analyses for the Light-Element Standards

- n-p scattering: N-N analysis goes up to 100 MeV; plan to to extend it to 200 MeV.
- ^{6}Li(n,t): ^{7}Li analysis gives excellent fits (χ^2/ν=1.36) to data up to 4 MeV.
- ^{10}B(n,α): ^{11}B analysis gives excellent fits (χ^2/ν=1.14) to data up to 1 MeV.
- Natural carbon: σ_{el} increased ~2% at 2 MeV, as already shown.



- Need accurate fission yields Y(A,Z,TKE) as a function of E_{inc}





D. Duke, PhD Thesis, LA-UR-15-28829 (2015)

- Also, ongoing theoretical work by A.J.Sierk (LANL)