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Title: Modeling Prompt Fission Neutrons and Their Uncertainties

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Intended for: Presented at the LANL-LLNL Fission Workshop
Feb. 3-5, 2009
Los Alamos, NM



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Abstract:

Prompt fission neutrons are important ingredients in the simulation of most nuclear-based technologies, including advanced reactors as envisioned in the Advanced Fuel Cycle Initiative. From a fundamental physics point of view, they also shed some light on the configurations of the nascent fission fragments near the scission point. In this talk, I will review the Los Alamos model used to calculate the average neutron multiplicity and spectrum in most evaluated data libraries. The methodology used to quantify uncertainties associated with the evaluated spectrum will be presented, and preliminary results in the case of $n(1 \text{ MeV}) + \text{Pu239}$ will be discussed. Finally, Monte Carlo simulations that describe in more details the emission mechanisms of prompt neutrons and gamma-rays are presented. Results for Cf252 , $n + \text{U235}$ and $n + \text{Pu239}$ reactions will be discussed.

Modeling Prompt Fission Neutrons and Their Uncertainties

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Post-Scission Physics

- Near scission, fission fragments are formed in *various configurations* (deformation, intrinsic excitation energies, pre-scission kinetic energy, ...)
- Very quickly ($\sim 10^{-20}$ s) the fragments separate and their deformation energies transform into excitation energies
- **How the available total excitation energy TXE is distributed among the two fragments remains an open question.**
- TXE is then evaporated through the emission of prompt neutrons and γ -rays



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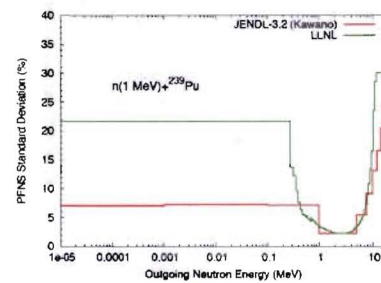
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Why it matters

- Fundamental understanding of fission physics
- Impact on AFCI advanced reactor sensitivity calculations
 - Simple estimates lead to sensitivities as large as for the cross-sections
- Impact on JEZEBEL critical assembly
 - Estimates of standard deviations from LLNL and JENDL-3.2 (Kawano, LANL)
 - Very simple testing of +/- one-sigma using JENDL and LLNL evaluated uncertainties
 - PARTISN calculations of k_{eff} (M.White, LANL) \rightarrow (-0.3%, +0.4%)!



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Prompt Fission Neutrons in Evaluated Libraries: The Los Alamos or Madland-Nix model

D.G. Madland and J.R. Nix,
Nucl. Sci. Eng. 81, 213-271 (1982)

Neutron energy spectrum in the laboratory frame:

$$N(E) = \frac{1}{2\sqrt{E_f}T_m^2} \int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} \sigma_c(\epsilon) \sqrt{\epsilon} d\epsilon \times \int_0^{T_m} k(T) T \exp(-\epsilon/T) dT$$

Fission fragment moving with a kinetic energy per nucleon E_f Energy-dependent cross-section for the inverse process of compound nucleus formation Triangular distribution of temperature from 0 to T_m

Assumptions:

- Average over fission fragments distribution
- Average over sequential neutron emissions
- Neutrons emitted from fully-accelerated fission fragments
- Thermal equilibrium at scission... and at time of neutron emissions



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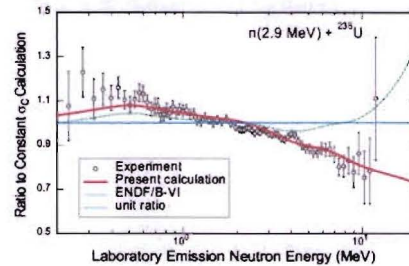
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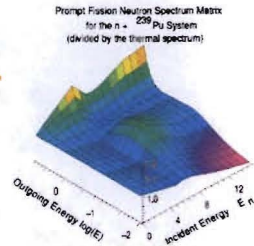


Los Alamos Model Successes... and limitations

- Great prediction for PFNS over a wide range of incident energies and isotopes



M.B. Chadwick *et al.*,
Nuclear Data Sheets 107, 2931-3060 (2006)



- No contributions from pre-equilibrium neutrons; scission neutrons?
- Hypothesis of thermal equilibrium at time of emission
- Computes averaged quantities only \rightarrow no correlations, distributions.
- No prescription for γ -ray spectrum



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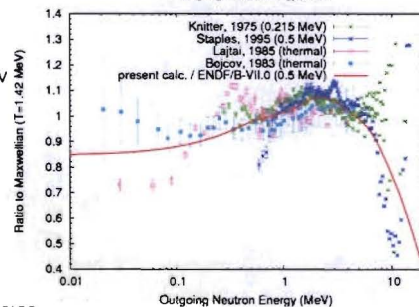
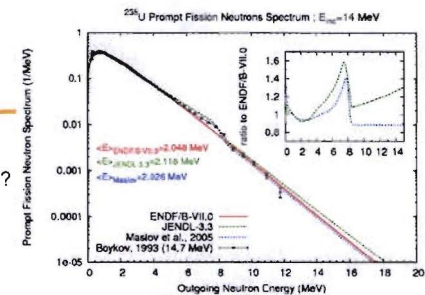
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Open Questions

- Fundamental physics**
 - Thermal equilibrium at time of emission?
 - Fission fragment yields and excitation energies?
- Pre-equilibrium neutrons**
- Low-energy outgoing neutrons**
 - Very little experimental data
 - Scission neutrons? Cf. Kornilov, Maslov
- Uncertainty Quantification**
 - How accurate?
- What about γ -rays?**
 - Important for existing and advanced reactors



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Uncertainty Quantification in the LA Model Framework

- **Uncertainties due to the model itself** – very difficult to assess without specific and accurate experimental data
- **UQ focusing on:**
 - Experimental uncertainties
 - Model parameters uncertainties
- **UQ Methodology**
 - **Assess uncertainties** (statistical + systematic) in experimental data sets
 - **Model parameters sensitivity calculations**
 - **Bayesian method** (Kalman filter) to combine both types of information
- **Benchmarking**
 - In critical assemblies
 - (n,2n) dosimetry reactions



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UQ of $n+^{239}\text{Pu}$: preliminary results

- **New LA model code**
 - Module written in Fortran 95
 - Tested successfully against D.G.Madland's own code and results
 - Reproduced successfully ENDF/B-VI.0 results
- **Experimental data sets included**
 - Knitter, 1975, $E_n=0.215$ MeV
 - Staples, 1995, $E_n=0.5$ MeV
- **Model sensitivity calculations performed with new code**
 - Varied parameters: $\langle \text{TKE} \rangle$, $\langle E_{\text{release}} \rangle$, a (1/MeV)
- **Preliminary covariance matrix obtained for $n(0.5 \text{ MeV})+^{239}\text{Pu}$ PFNS**



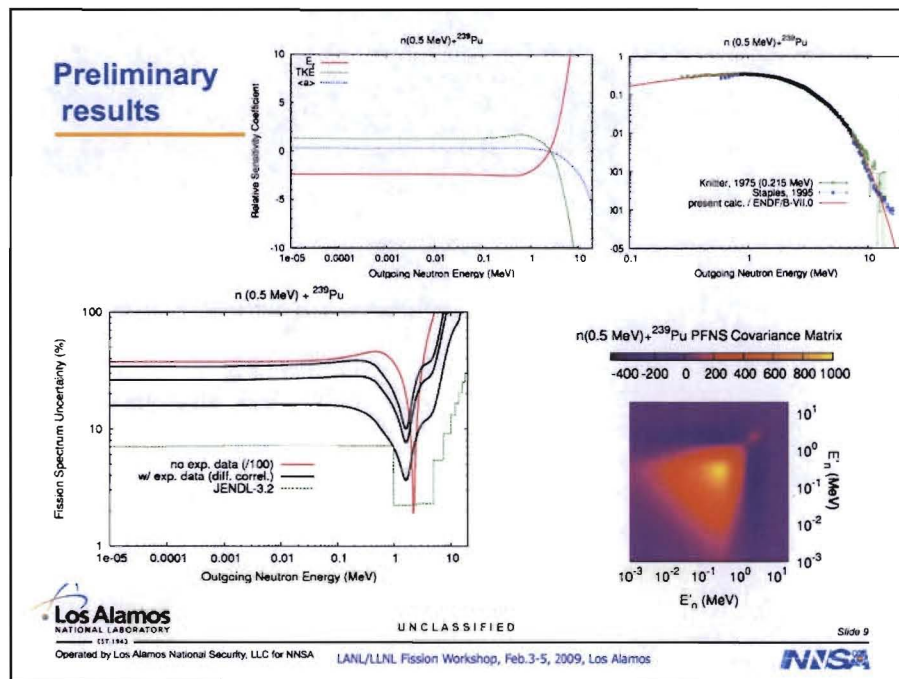
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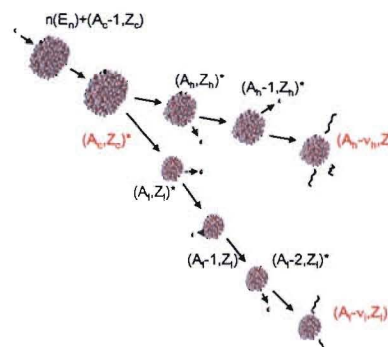




Beyond the Los Alamos Model: Hauser-Feshbach Description of the Emission of Neutrons

- Follow cascading neutron emissions event-by-event
- Samples the entire fission fragments distribution $Y(A,Z,KE)$
- Provides
 - Detailed neutron and γ -ray spectra
 - Average multiplicities and multiplicity distributions
 - Angular and energy correlations: n-n, γ - γ , n-FF, etc.
 - Etc.

on an event-by-event basis



Input Ingredients

- Neutrons emitted from a Weisskopf distribution at temperature T
- $\sigma_c(\epsilon)$ calculated with the Koning-Delaroche global optical potential (2003)
- Most probable charge from known deviations from UCD
- Nuclear masses from Audi-Wapstra (2003)
- Level density from Gilbert-Cameron-Ignatyuk formula, and RIPL-2 systematics
- Fission fragment yields $Y(A, TKE)$ from experimental data
- Plus **one model parameter R_f** to distribute excitation energy in light and heavy fragments (in case of multi-modal fission, one parameter per fission mode)



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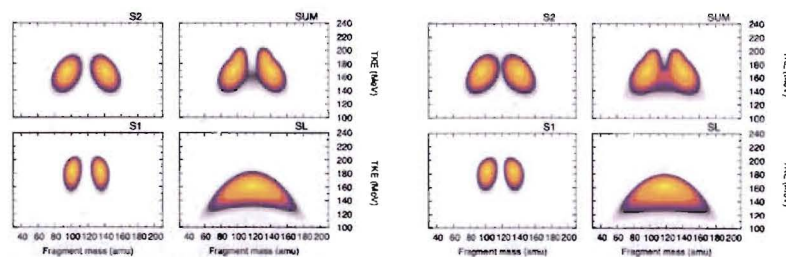
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Application: $n+^{235}\text{U}$ ($E_{\text{inc}}=0.5$ to 6 MeV)

- Experimental yields $Y(A, TKE)$ from Habsch data (Geel, 2006)
- Decomposition in Brosa fission modes (S1, S2, and SL)



1.0 MeV

6.0 MeV



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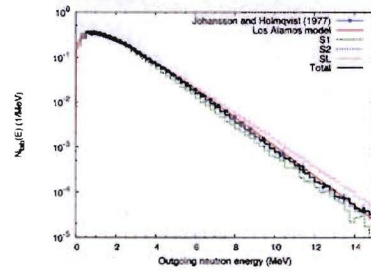
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Main results



Calculated spectrum slightly too soft in the 6-10 MeV energy region

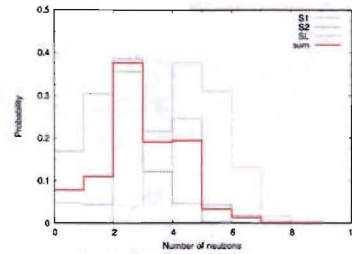
$$\langle \nu \rangle_{\text{calc}} = 2.47; \langle \nu_f \rangle_{\text{calc}} = 1.40; \langle \nu_h \rangle_{\text{calc}} = 1.07$$

Müller (1984) $\langle \nu \rangle = 2.46; \langle \nu_f \rangle = 1.44; \langle \nu_h \rangle = 1.02$
 Nishio (1998, n_{th}) $\langle \nu \rangle = 2.47; \langle \nu_f \rangle = 1.42; \langle \nu_h \rangle = 1.01$

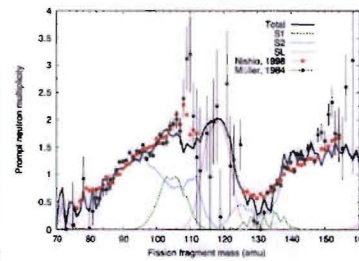
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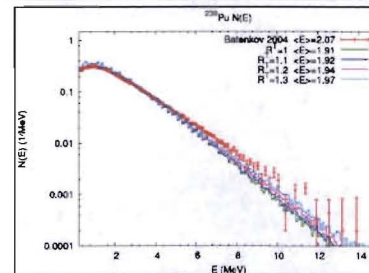
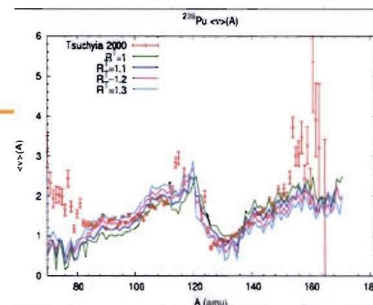
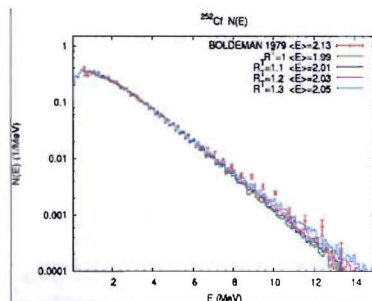
Not only $\langle \nu \rangle$,
but also $P(\nu)$ and $\langle \nu \rangle(A)$



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Other Studies

$^{252}\text{Cf}(sf)$ and $n_{th} + ^{239}\text{Pu}$



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What's next?

■ Theory

- Expand Los Alamos model to include pre-equilibrium component and R_T parameter
- Advanced Modeling of Prompt fission neutrons and γ -rays spectra
 - Full Hauser-Feshbach calculations
 - Uncertainty quantification
 - Fundamental calculations of $Y(Z,A,E^*,J)$
 - **Goal: reach level of accuracy of current Los Alamos model evaluations**
- + Correlations, distributions

■ Experiment

- Need for more detailed data: correlations, distributions
- Accurate assessment of uncertainties (and correlations)

■ Evaluation / Benchmarking

- Inclusion of clean integral data (e.g., JEZEBEL) in the evaluation procedure
- Quick feedback



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