Uncertainty Quantification on Prompt Fission Neutrons Spectra

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Why do we need it?

- **A small uncertainty on the Prompt Fission Neutron Spectrum (PFNS) can have a significant impact in integral data simulations**

  - JAEA Studies (1999+):
    - Sensitivity analyses performed by Ishikawa et al.
    - Uncertainties in the Madland-Nix model calculations estimated by Ohsawa and Kawano using the KALMAN code
    - ERRORJ can handle PFNS covariance matrix processing

  - LANL study of Jezebel Pu sphere (M.C.White, 2008);
    PARTISN calculations of k_{eff} with uncertainties on ^{239}Pu χ-matrix
    ➠(-0.3%;+0.4%) !!

  - Conclusions from OECD/WPEC Subgroup 26 chaired by M.Salvatores.
    Report G.Aliberti, M.Salvatores *et al.* (2008).

Methodology

- **Approach similar to what LANL used for cross-section covariance matrices evaluations**
  - Sensitivity of the calculated results to model parameters
  - Assessment of experimental uncertainties
  - Combine both types of information with a Kalman filtering technique
- **The Los Alamos or Madland-Nix model is used to compute the prompt fission neutron spectrum** -- a completely new and modern version of Madland's codes was implemented.
- **The KALMAN code [T.Kawano] is used to perform the Kalman filter.**

"An estimation of the uncertainty associated with an evaluated data must be obtained within the exact same approach that led to the evaluation of the data in the first place."

The Los Alamos model of Prompt Fission Neutrons Spectrum

- The **neutron energy spectrum *N(E)* in the laboratory frame** for a fission fragment moving with a kinetic energy per nucleon E_f reads

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

where k(T) is the temperature-dependent normalization constant

$$k(T)^{-1} = \int_0^{\infty} \sigma_c(\epsilon)\epsilon exp(-\epsilon/T) d\epsilon.$$

- Considering the most probable fragmentation only, and assuming $<\nu_L>=<\nu_H>$,

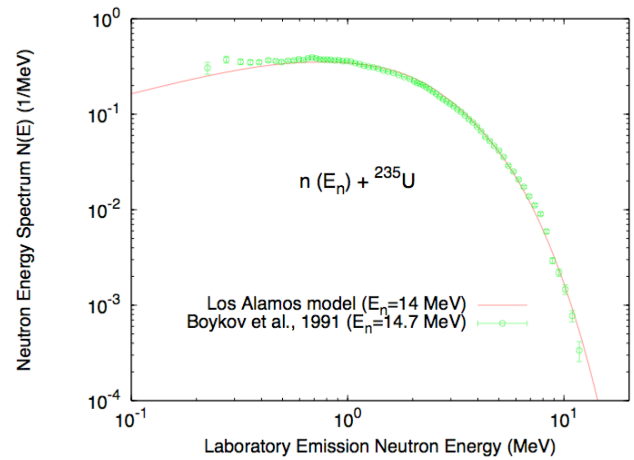
$$N(E) = \frac{1}{2}\left(N_L(E) + N_H(E)\right)$$

- Generalization to **multi-chance fission**:

$$N(E) = \sum_i P_f^i \times \left(\sum_{j=1}^{i-1} \phi_j(E) + \overline{\nu}_i N_i(E) \right) / \sum_i P_f^i \times (i - 1 + \overline{\nu}_i)$$

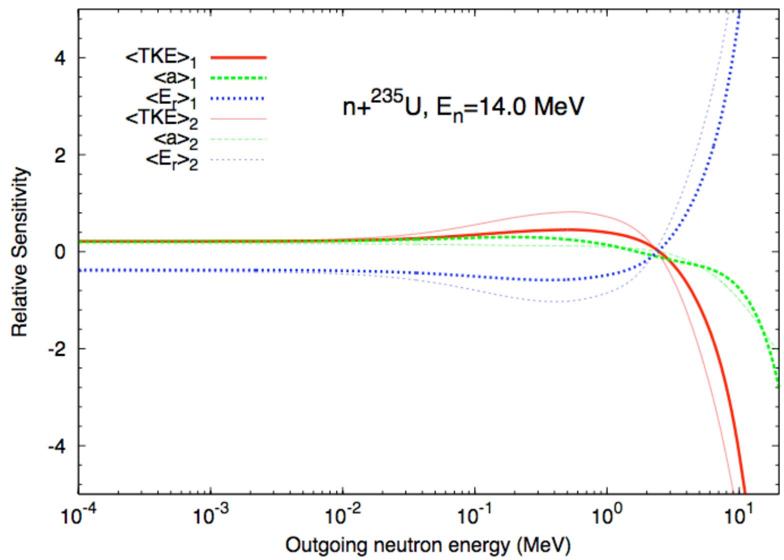
Sensitivity to Model Parameters

- **Central values chosen to reproduce ENDF/B-VII.0 results**
- **Initial guesses of uncertainty bands**



n+^{235}U

Parameter	Value (MeV)	Uncertainty (%)
$< TKE >_1$	171.80	2.0
$< TKE >_2$	171.95	2.0
$< TKE >_3$	172.10	2.0
$< E_r >_1$	186.98	8.0
$< E_r >_2$	188.946	8.0
$< E_r >_3$	188.971	8.0
a_1	236/11.	9.0
a_2	235/11.	9.0
a_3	234/11.	9.0



Experimental Data

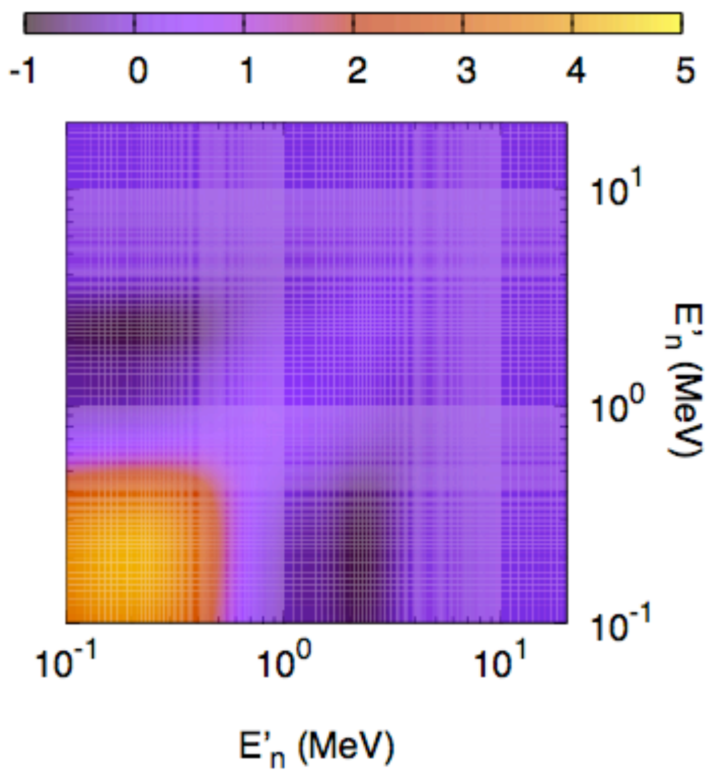
- **n+^{235}U**
  - P.I.Johansson & B.Holmqvist, *Nucl. Sci. Eng.* **62**, 695 (1977). E_n=0.53 MeV.
  - G.Boykov *et al.*, *Sov. J. Nucl. Phys.* **53**, 392 (1991). E_n=2.9 and 14.7 MeV.
- **Statistical uncertainties obtained from experimental work**
- **Systematic uncertainties:** for now, simply estimated with a 50% correlation factor.

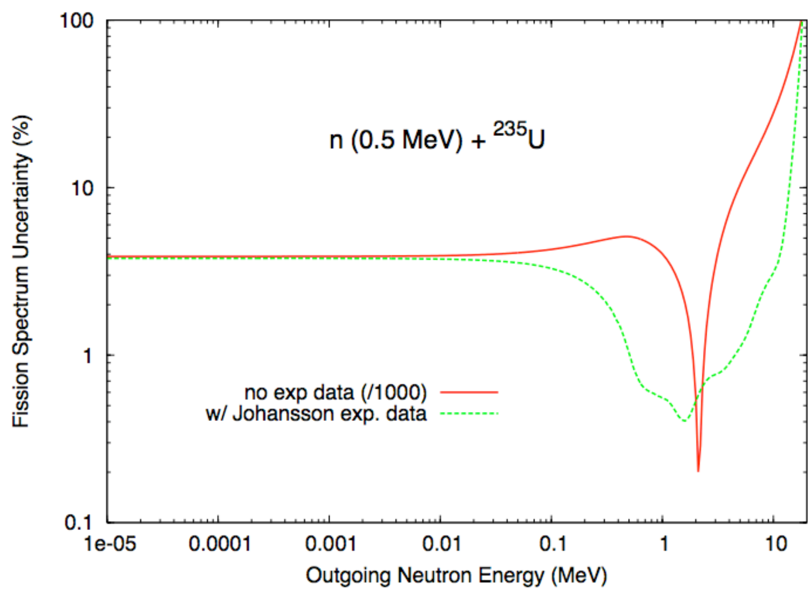
Kalman Filter Equations

$$
\begin{aligned}
\mathbf{m_1} &= \mathbf{m_0} + \mathbf{PC}^t\mathbf{V}^{-1}(\phi - f(\mathbf{m_0})) \\
&= \mathbf{m_0} + \mathbf{XC}^t(\mathbf{CXC}^t + \mathbf{V})^{-1}(\phi - f(\mathbf{m_0})) \\
\mathbf{P} &= (\mathbf{X}^{-1} + \mathbf{C}^t\mathbf{V}^{-1}\mathbf{C})^{-1} \\
&= \mathbf{X} - \mathbf{XC}^t(\mathbf{CXC}^t + \mathbf{V})^{-1}\mathbf{CX}.
\end{aligned}
$$

- **Prior:**
  - $\mathbf{m}_0$: prior vector of model parameters
  - **X**: prior model parameter covariance matrix (diagonal)
- **Posterior:**
  - $\mathbf{m}_1$: posterior vector of model parameters
  - **P**: posterior parameter covariance matrix
  - **F**: evaluated covariance matrix for PFNS
- **Calculation & Experiment**
  - $f(\mathbf{m}_0)$: calculated spectrum using *prior* parameter values
  - **C**: calculated sensitivity matrix
  - **V**: experimental covariance matrix

Preliminary Results: n(0.5 MeV)+^{235}U





Conclusions & Perspectives

- **All tools now in place to produce PFNS covariance matrices for ENDF/B-VII.1**
- **First applied successfully to the n+^{235}U reaction.**
- **In the near future:**
  - Inclusion of all model parameter uncertainties; some like fission probabilities, inverse compound formation cross section, … were not studied in this preliminary work.
  - Application to the three major actinides: ^{235,238}U and ^{239}Pu (➟ ENDF/B-VII.1)
  - ENDF format output for use in applications
- **Longer term:**
  - Address Los Alamos model limitations by developing a more comprehensive approach to the emission of neutrons from excited fission fragments.
  - A more detailed model would also provide a more detailed and robust uncertainty assessment.