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Title: Introducing Nuclear Data Evaluations of Prompt Fission Neutron Spectra

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Introducing Nuclear Data Evaluations of Prompt Fission Neutron Spectra

6/23/2015 T-2 Seminar

D. Neudecker

XCP-5, XCP Division, LANL, work performed in T-2

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M.C. White, M.E. Rising, J.P. Lestone, D. Vaughan (XCP)
R.C. Haight, T.N. Taddeucci, H.Y. Lee (P-27)
T. Burr (CCS-6), R. Capote (IAEA), D.L. Smith (ANL)

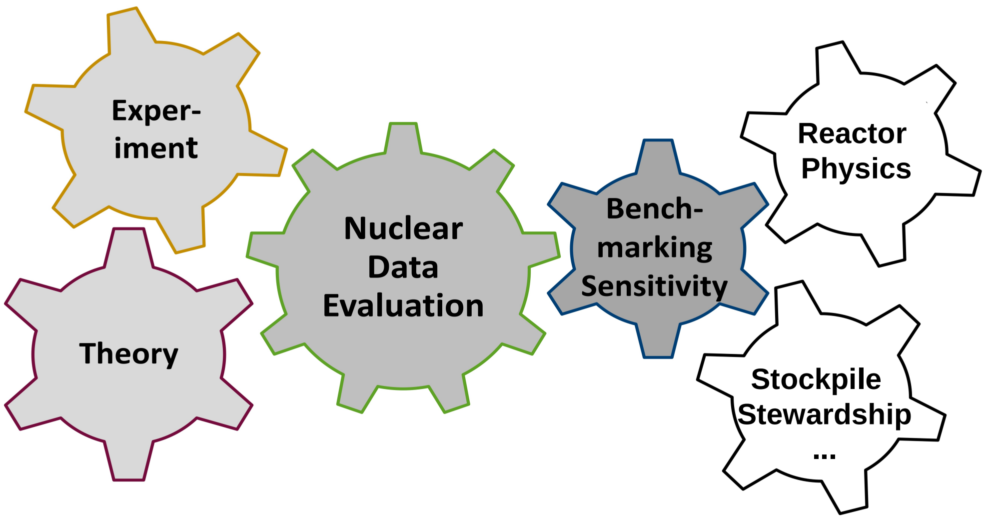
Abstract

Nuclear data evaluations provide recommended data sets for nuclear data applications such as reactor physics, stockpile stewardship or nuclear medicine. The evaluated data are often based on information from multiple experimental data sets and nuclear theory using statistical methods. Therefore, they are collaborative efforts of evaluators, theoreticians, experimentalists, benchmark experts, statisticians and application area scientists. In this talk, an introductions is given to the field of nuclear data evaluation at the specific example of a recent evaluation of the outgoing neutron energy spectrum emitted promptly after fission from ^{239}Pu and induced by neutrons from thermal to 30 MeV.

Evaluation of the ^{239}Pu Prompt Fission Neutron Spectrum and Covariances

- Introduction
  - What is nuclear data evaluation?
  - What is a PFNS?
- The ^{239}Pu PFNS evaluation
  - Experimental information …
  - Model information …
- Summary and Future Activities

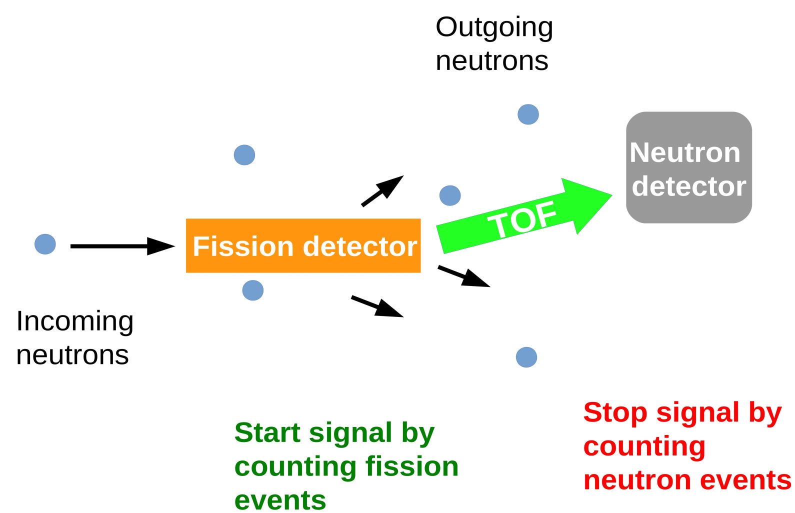
Introduction



What is 'nuclear data evaluation'?

What is a prompt fission neutron spectrum (PFNS)?

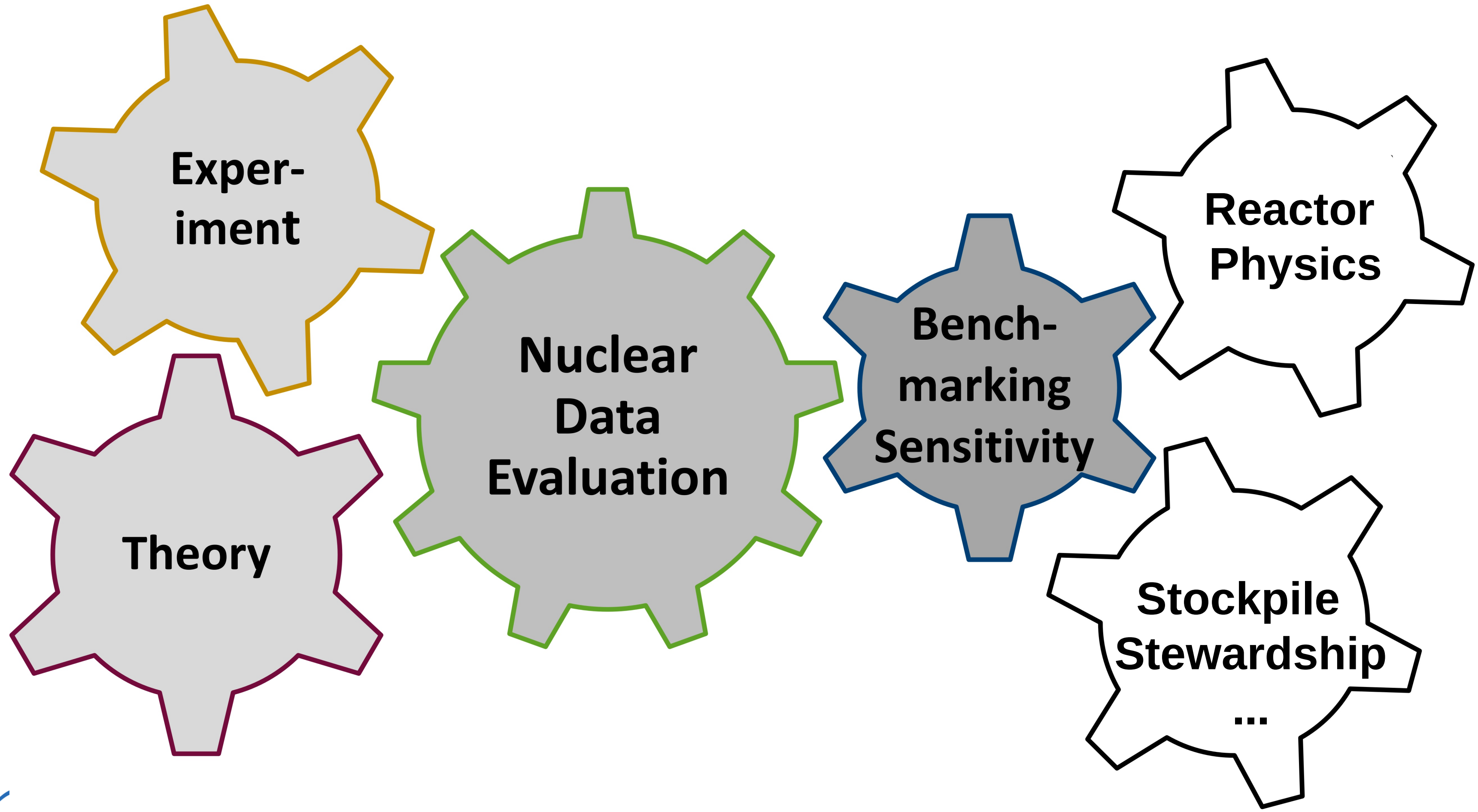
Why do we need it?



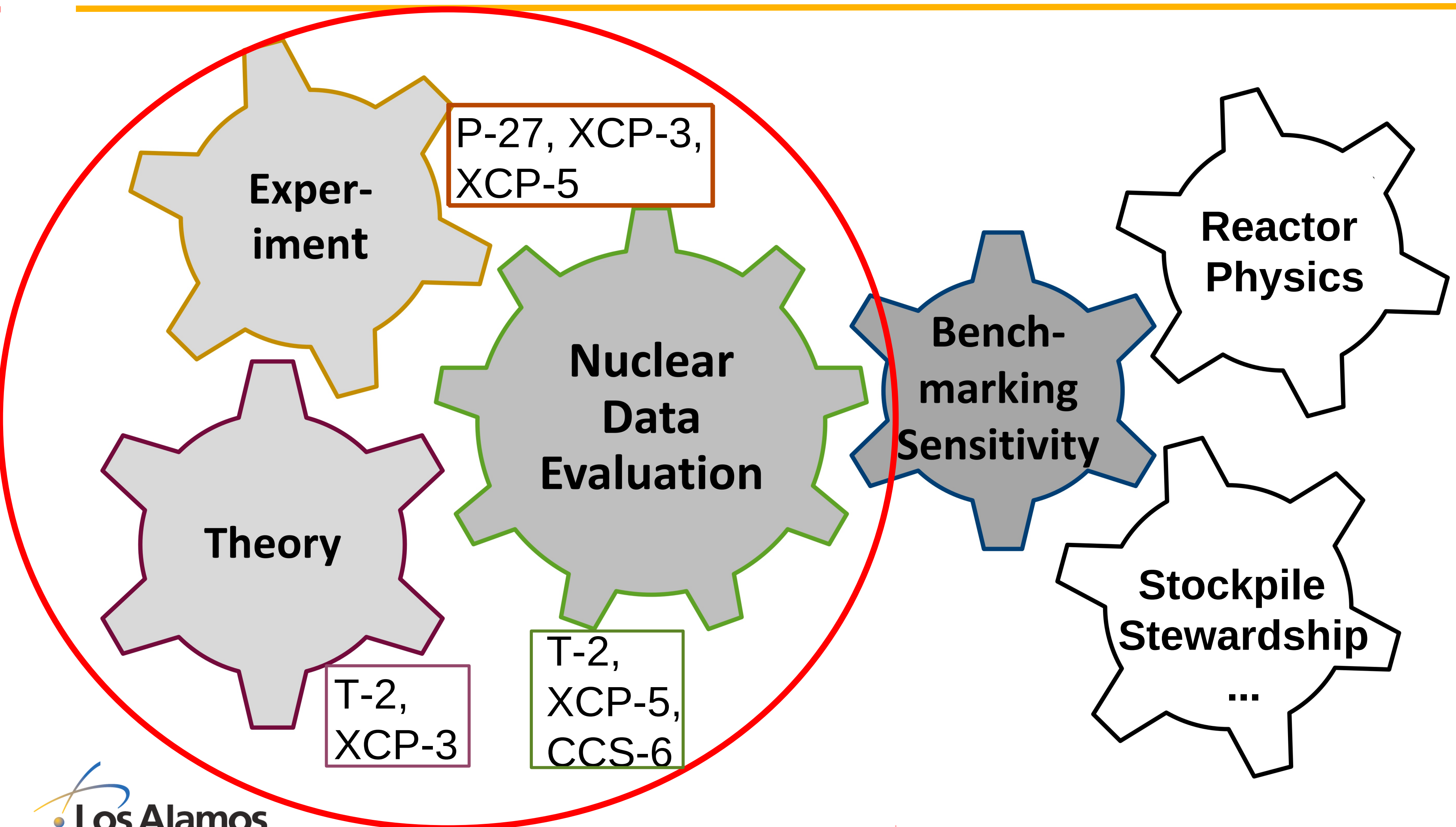
Introduction

What is 'nuclear data evaluation'?

Nuclear data evaluations provide recommended data for nuclear applications.



Nuclear data evaluations often contain model and experimental information.

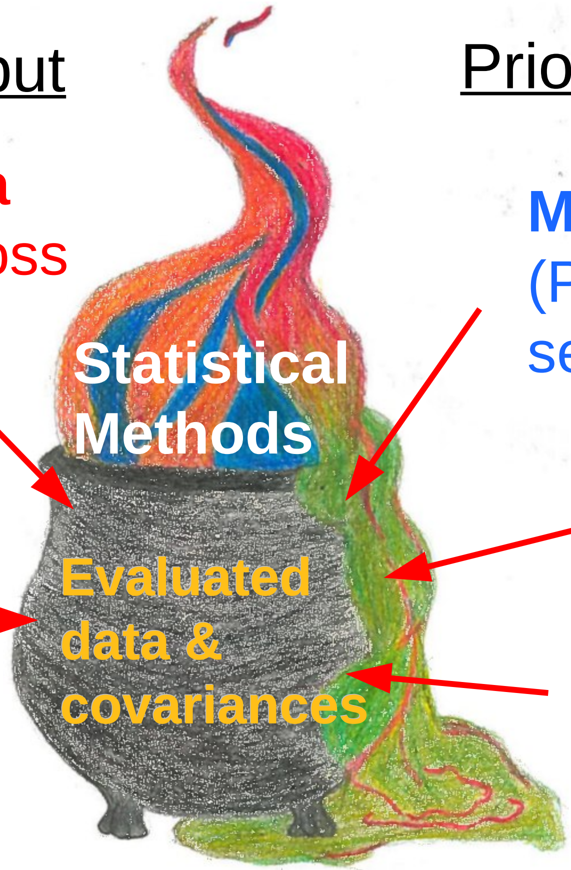


Nuclear data evaluations combine model predictions and experimental information.

<u>Experimental Input</u>

Experimental data
(PFNS, <TKE>, cross sections, etc.)

Experimental covariances



<u>Prior (Theoretical) Input</u>

Model predicted data
(PFNS, <TKE>, cross sections, etc.)

Parameter Uncertainties

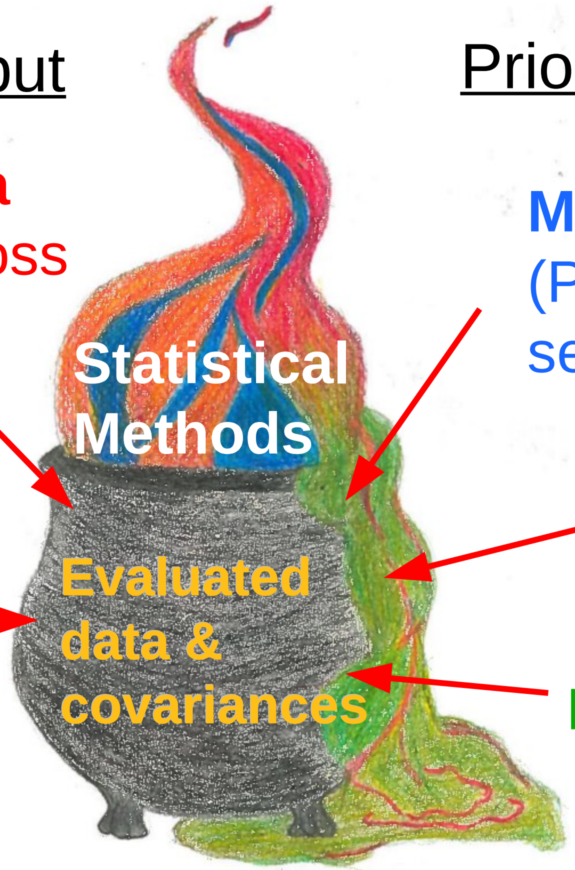
Model Defects

Nuclear data evaluations combine model predictions and experimental information.

<u>Experimental Input</u>

Experimental data
(PFNS, <TKE>, cross sections, etc.)

Experimental covariances



<u>Prior (Theoretical) Input</u>

Model predicted data
(PFNS, <TKE>, cross sections, etc.)

Parameter Uncertainties

Model Defects

D. Neudecker, R. Capote, H. Leeb, NIMA **723**, 163 (2013).

Often Generalized Least Squares algorithms are used for the evaluation.

$$\underline{\phi}^{post} = \underline{\phi}^{M} + \mathbf{Cov}^{post}\mathbf{S}^{+}(\mathbf{Cov}^{x})^{-1}\left(\underline{\phi}^{x} - \mathbf{S}\underline{\phi}^{M}\right),$$

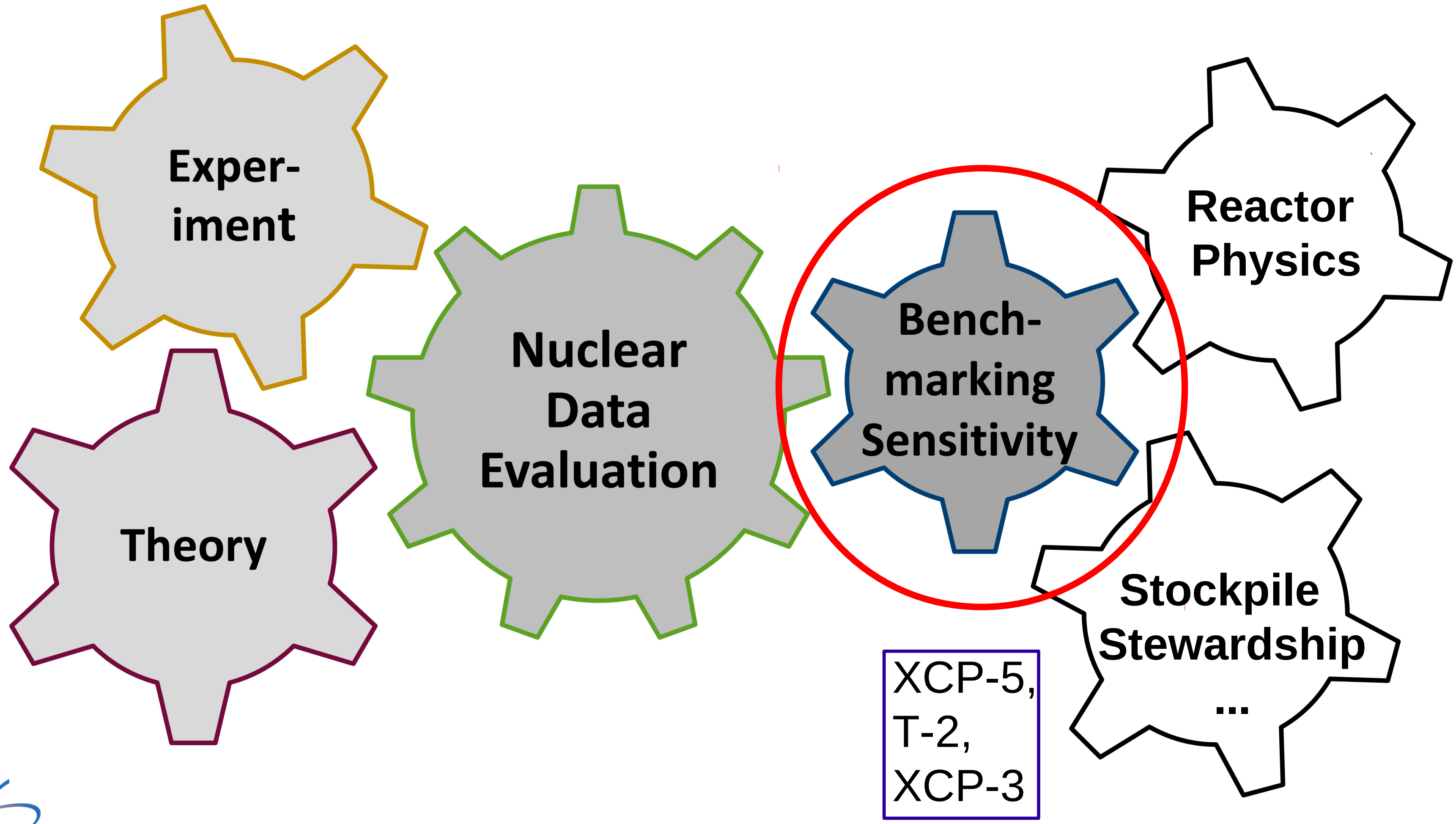
$$\mathbf{Cov}^{post} = \mathbf{Cov}^{M} - \mathbf{Cov}^{M}\mathbf{S}^{+}\left(\mathbf{S}\mathbf{Cov}^{M}\mathbf{S}^{+} + \mathbf{Cov}^{x}\right)^{-1}\mathbf{S}\mathbf{Cov}^{M}$$

This is a standard statistical algorithm … but it assumes:

- Experimental data are normally distributed.
- Model data are normally distributed.

?

Benchmark tests compare computed benchmarks to integral experiments.



The effective multiplication factor of critical assemblies - good benchmark for ^{239}Pu PFNS.

The **Jezebel critical assembly** consists of two ^{239}Pu half spheres and is used to study the **effective multiplication factor k_{eff}**:

$k_{eff} = 1 \rightarrow$ critical $\quad k_{eff} < 1 \rightarrow$ sub-critical $\quad k_{eff} > 1 \rightarrow$ super-critical

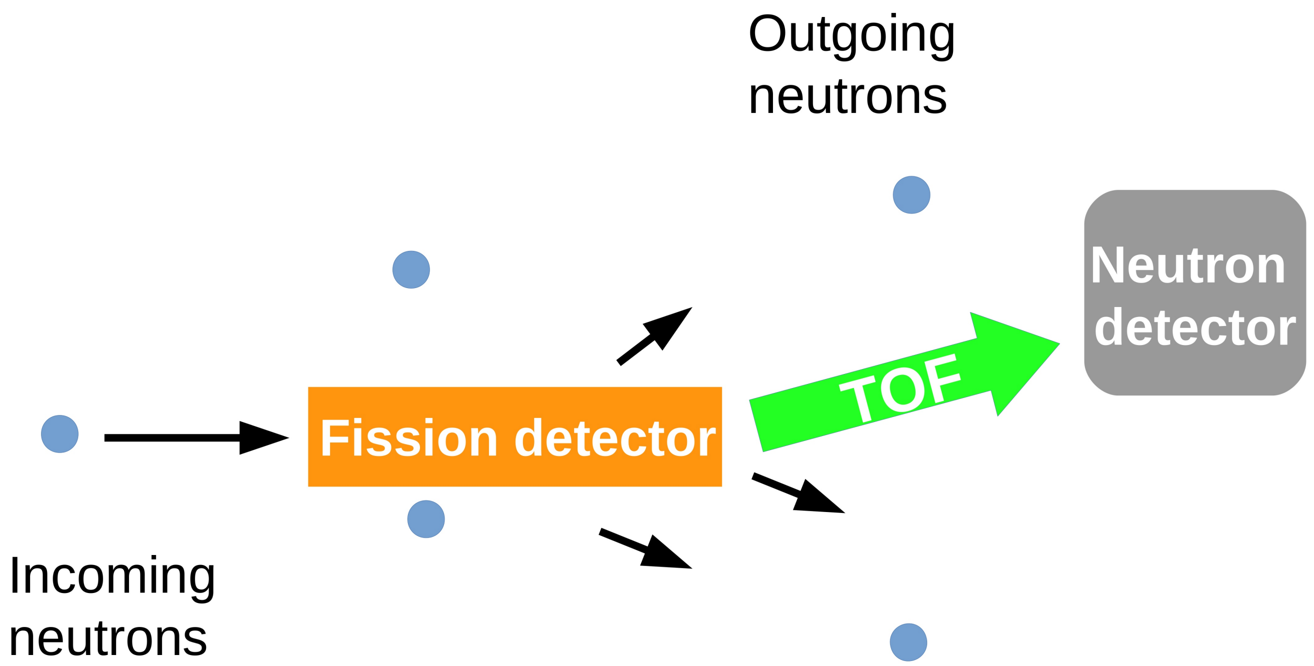
The Boltzmann Eqs. **simulate this assembly using nuclear data.** These simulations help us **benchmark** nuclear data relative to measured values of k_{eff}.

Introduction

What is a prompt fission neutron spectrum (PFNS)?

Why do we need it?

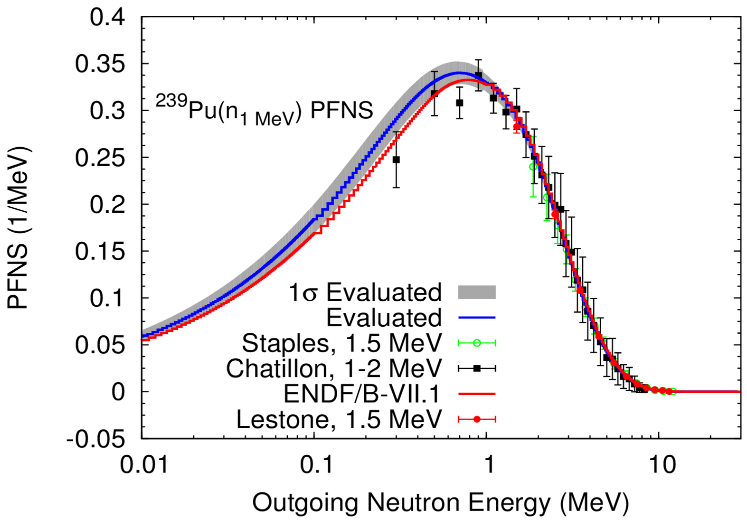
A PFNS gives the energy distrib. of neutrons emitted after scission & before β-decay

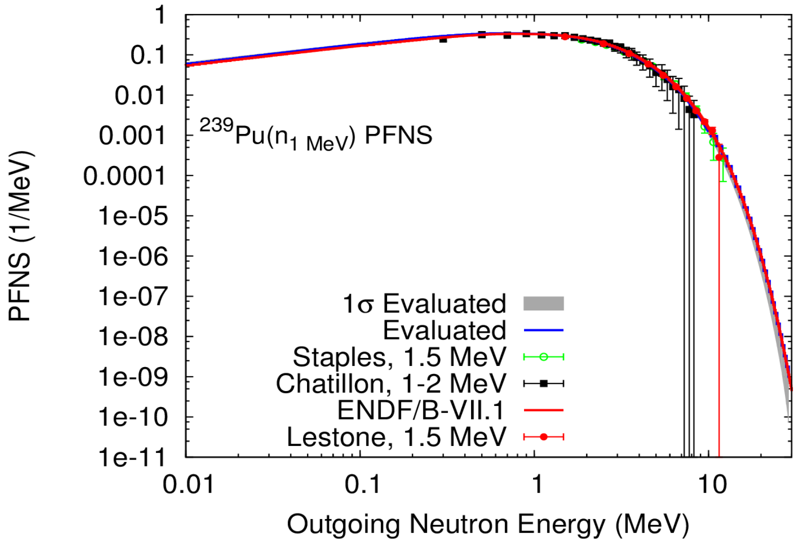


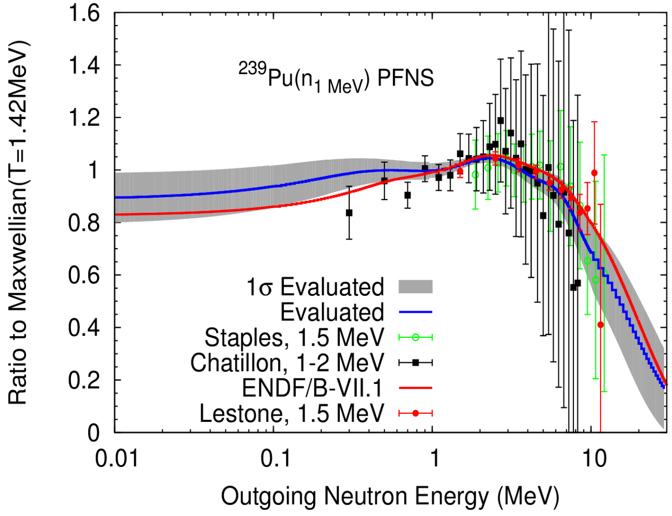
Start signal by counting fission events

Stop signal by counting neutron events

A PFNS covers many orders of magnitudes.

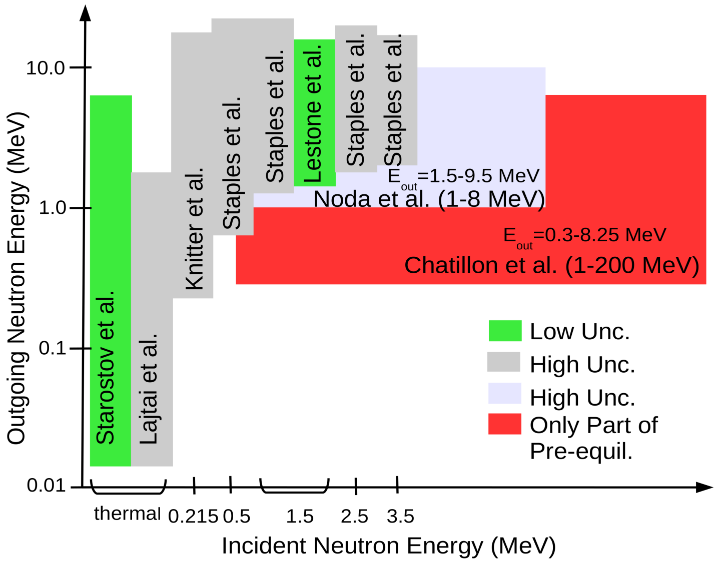






$$\mathrm{Maxw} \propto \sqrt{E}\exp\left(-E/T\right)$$

The ^{239}Pu PFNS Evaluation

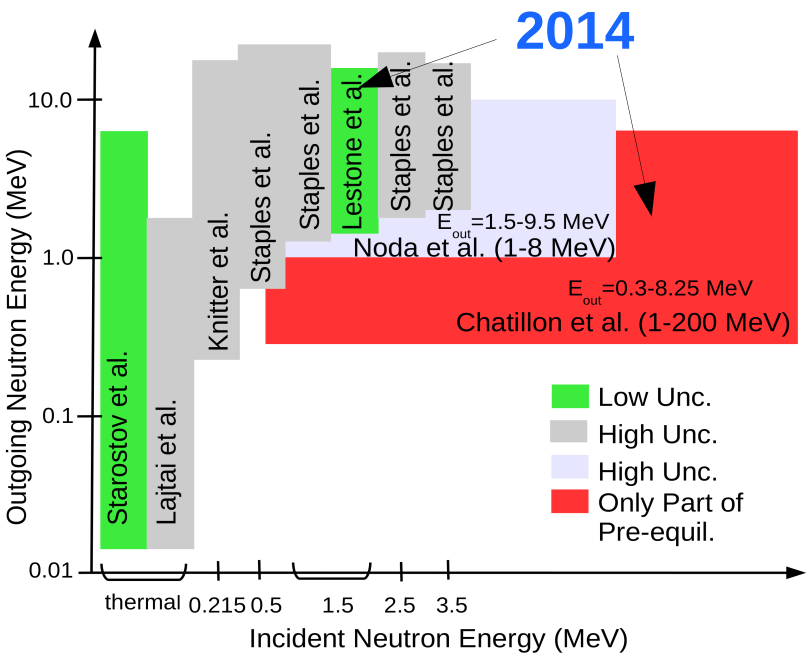


Why a new ^{239}Pu PFNS evaluation?

A new ^{239}Pu PFNS evaluation was undertaken due to new exp. & model info.

P. Talou et al., Nucl. Science Eng. **166,** 254 (2010) provided an evaluation for E_{inc} = 500 keV with covariances, since then:

Experiment



Model

- Not all physics processes considered for higher E_{inc} in current library.
- New parametrizations of important model parameters are available.

Improved ^{239}Pu PFNS for follow-up of ENDF/B-VII.1, IAEA CRP & CIELO → applications:

- Development of innovative nuclear reactors (Generation IV-reactors, small and modular reactors)
- Dosimetry
- Global Security
- Stockpile stewardship
- Non-proliferation …

Not only mean values but also covariance matrices are needed!

The ^{239}Pu PFNS Evaluation: Experimental Data and Uncertainties

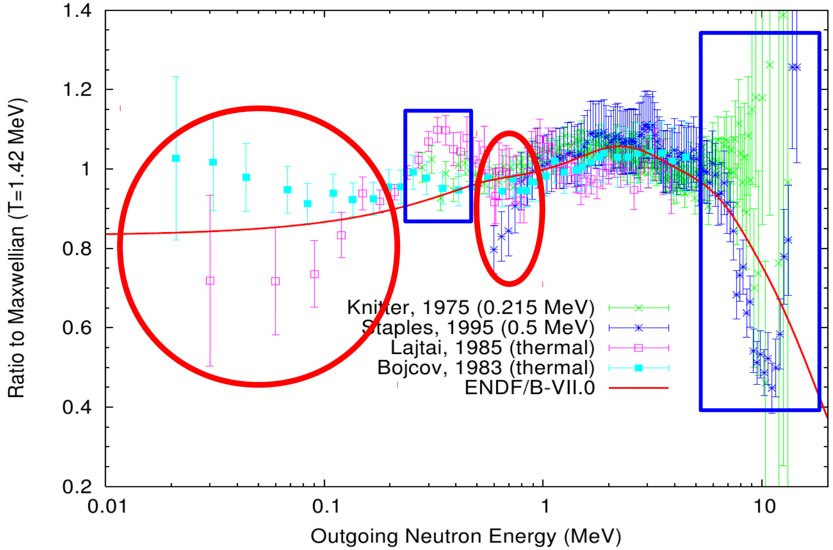
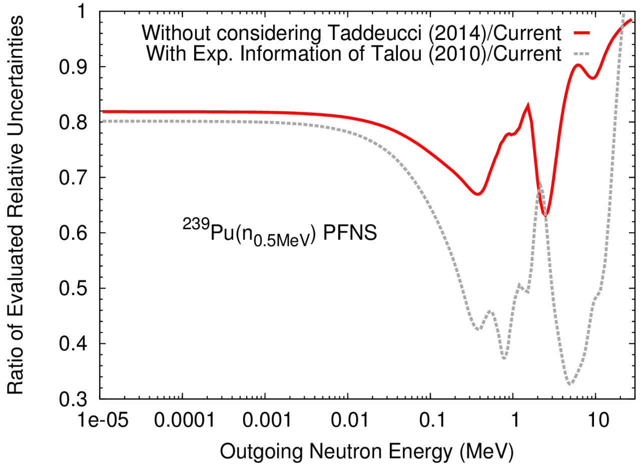


FIGURE 2. Same as Fig. 1 but shown as a ratio to a Maxwellian at temperature T=1.42 MeV.

Why did we look in detail in exp. data and uncertainties?

Does an improved exp. UQ matter?



The ^{239}Pu PFNS Evaluation: Experimental Data and Uncertainties

Why did we look in detail in exp. data and uncertainties?

Differential experimental data show discrepancies, which are partly larger than 1σ error bars!

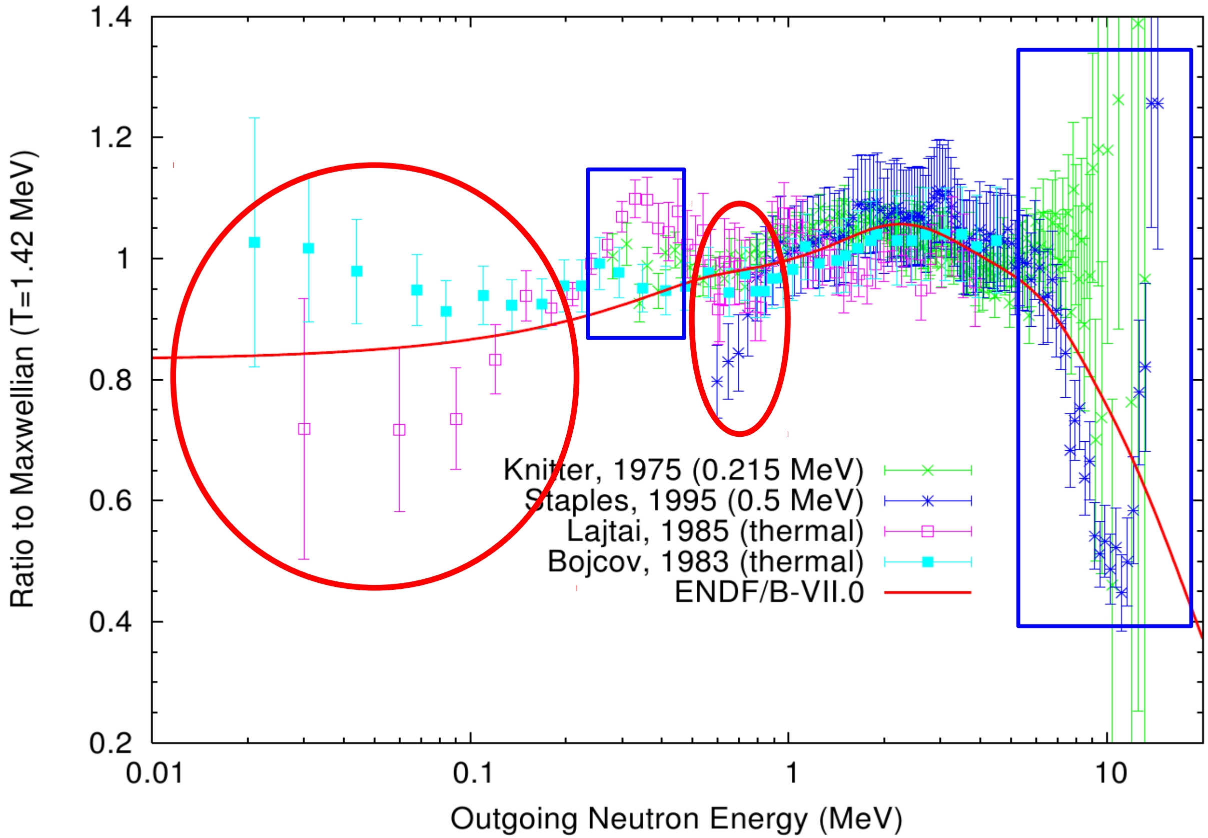


FIGURE 2. Same as Fig. 1 but shown as a ratio to a Maxwellian at temperature T=1.42 MeV.

Taken from P. Talou et al. LA-UR-19-00646, published in NSE **166,** 254 (2010).

Evaluated uncertainties were surprisingly low and partly attributed to simplified exp. UQ.

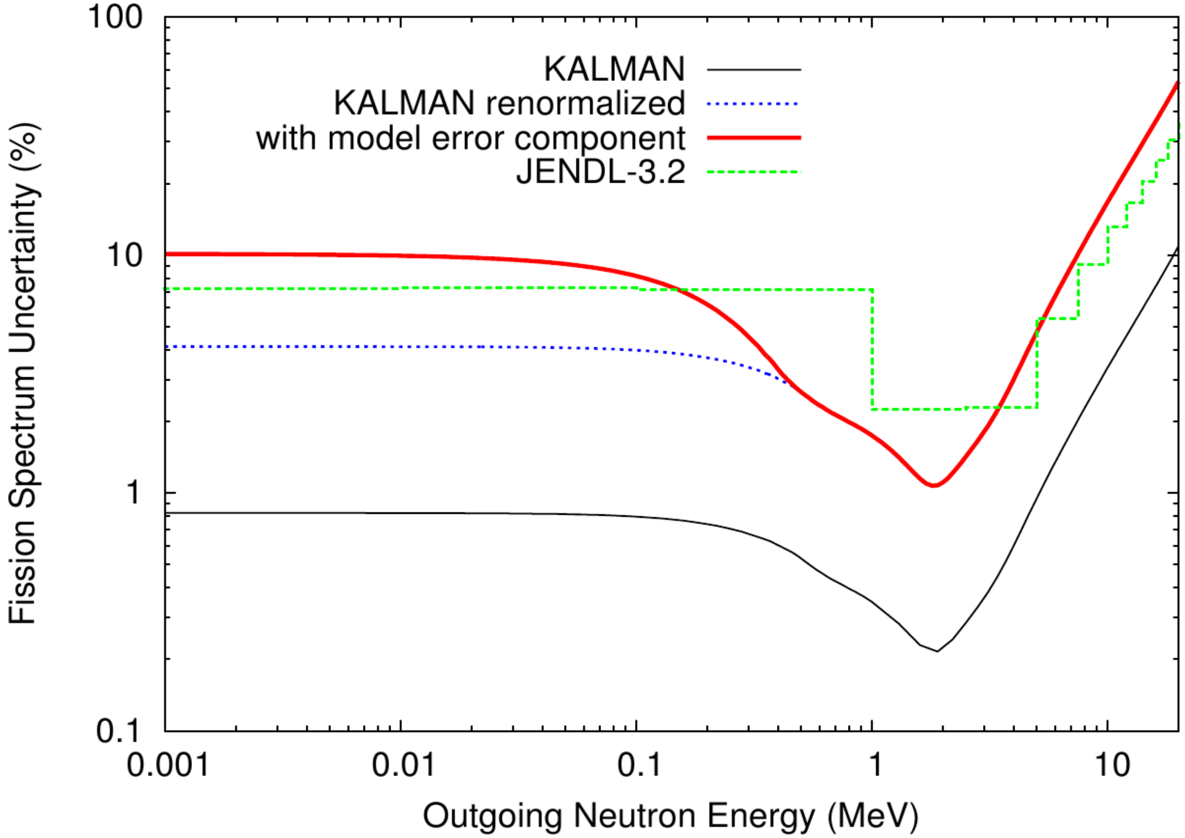
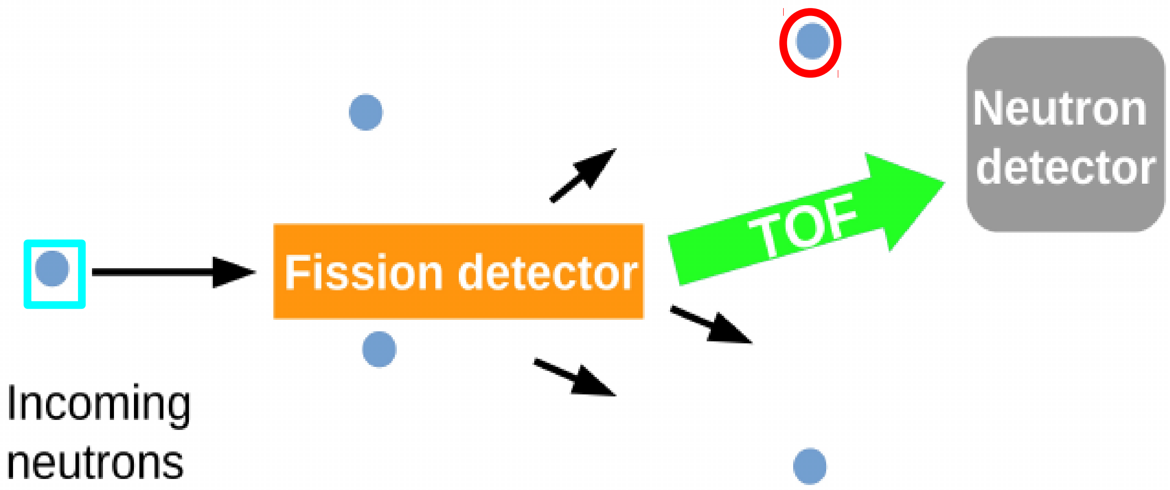


FIGURE 4. Calculated standard deviations for the evaluated PFNS of n(0.5 MeV)+^{239}Pu. See text for details.

Taken from P. Talou et al. LA-UR-19-00646, published in NSE **166,** 254 (2010).

Experimental uncertainties are estimated by partitioning them into their respective sources.



$$Cov^{\exp} = Cov^{Count.\,Stat.} + Cov^{Backgd.} + Cov^{Mult.\,Scatt} + Cov^{TOF} + Cov^{Det.\,Eff} + \ldots$$

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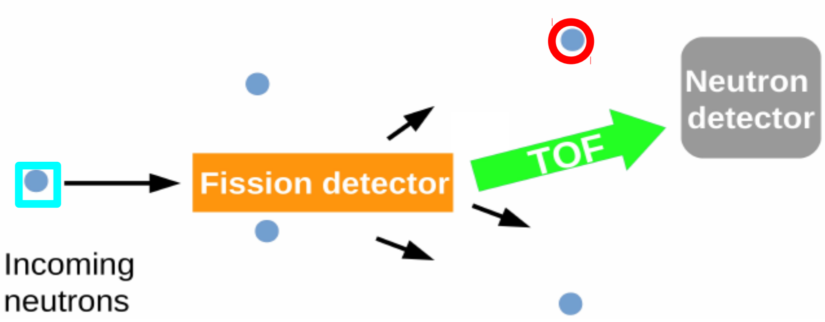
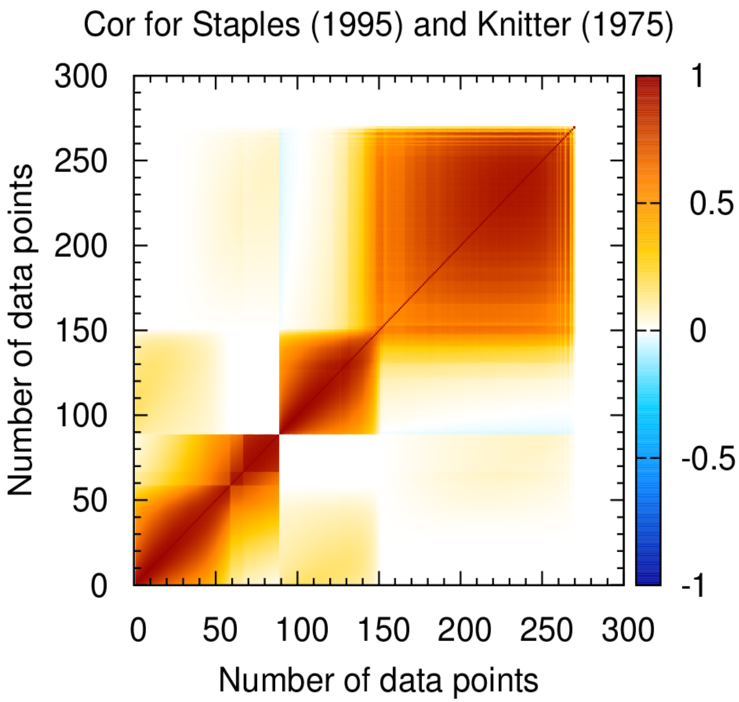


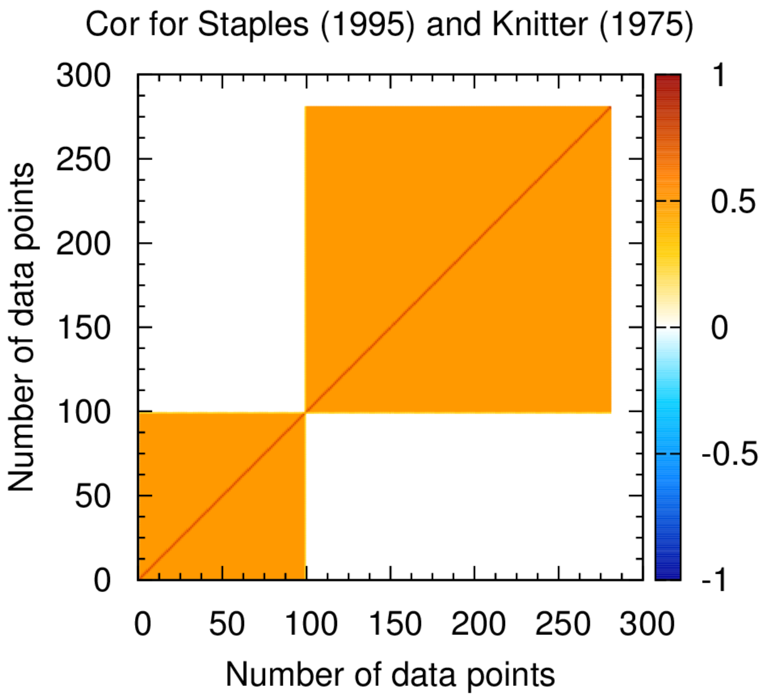
$$Cov^{exp} = Cov^{Count.Stat.} + Cov^{Backgd.} + Cov^{Mult.Scatt.} + Cov^{TOF} + Cov^{Det.Eff} + \ldots$$

- Facilitates estimation of reasonable correlations.
- Additional uncertainty sources can be added easily.
- Estimate of uncertainties between different experiments more transparent.

Experimental correlation matrices differ distinctly.

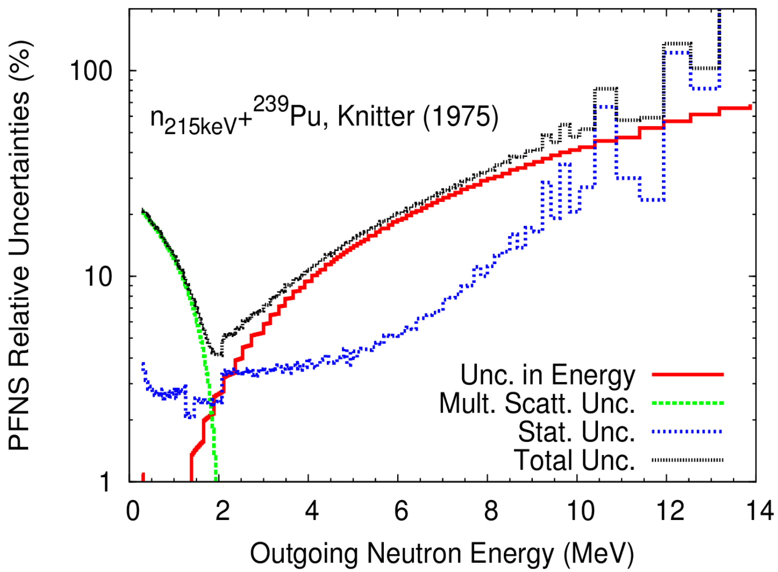


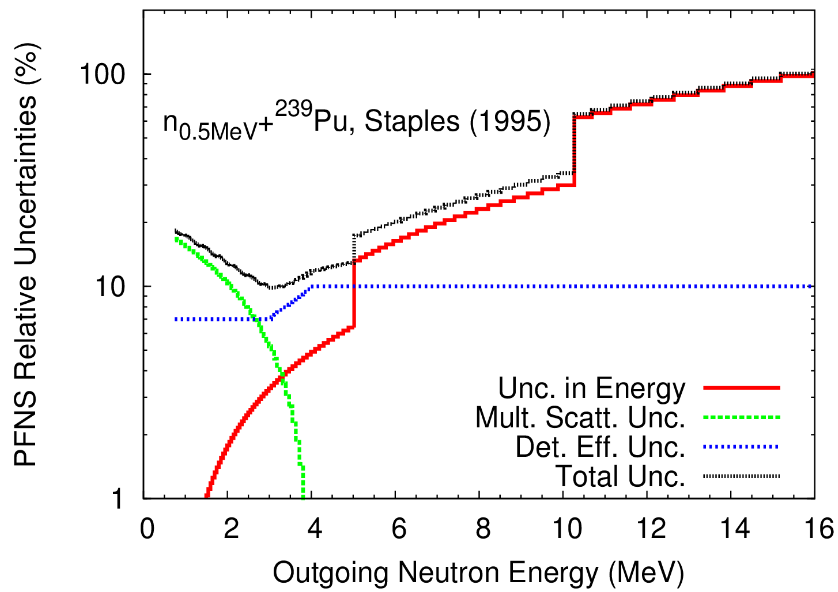
This Work



Talou (2010)

We added uncertainties for recently discovered under-estimated effects, e.g., multiple scattering.

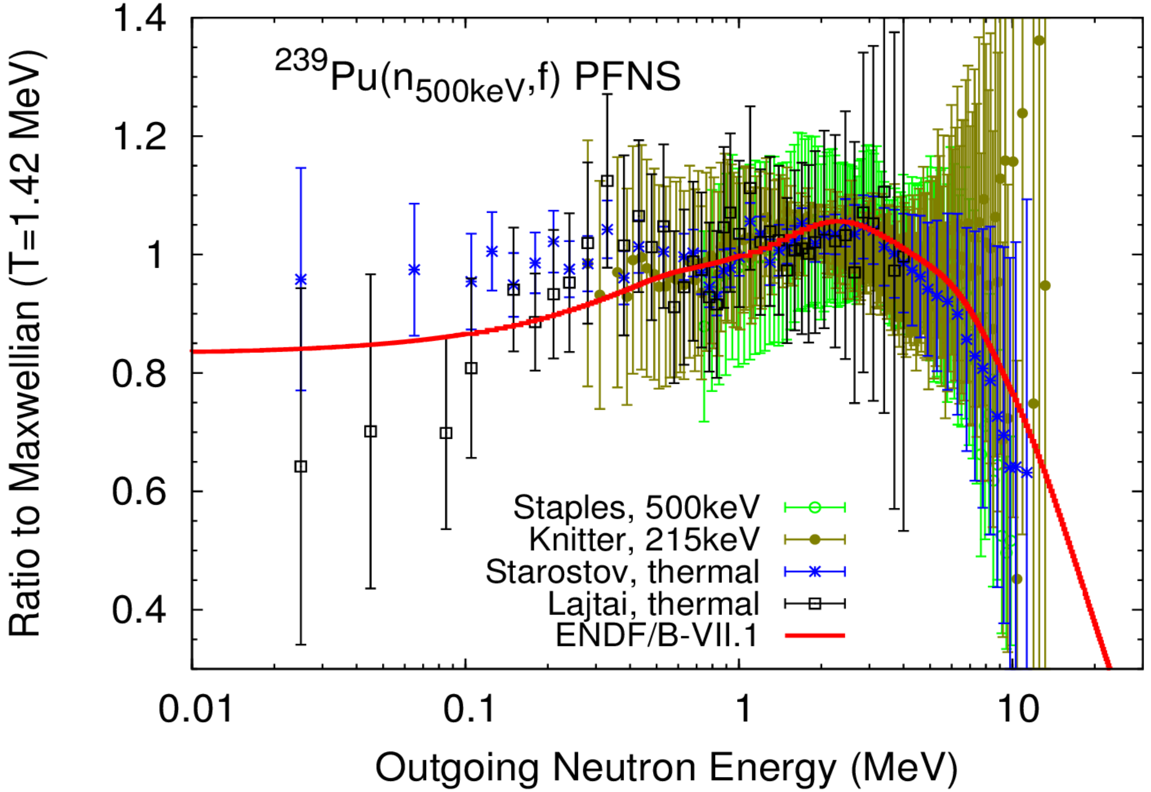




Multiple scattering, deconvolution and background unc. were estimated according to:

T.N. Taddeucci et al., Nucl. Data Sheets **123**, 135 (2015), CW2014 Proceeding.

The 1σ error-bars of most of the data overlap considering uncertainties of additional effects.



But better data is needed ?!

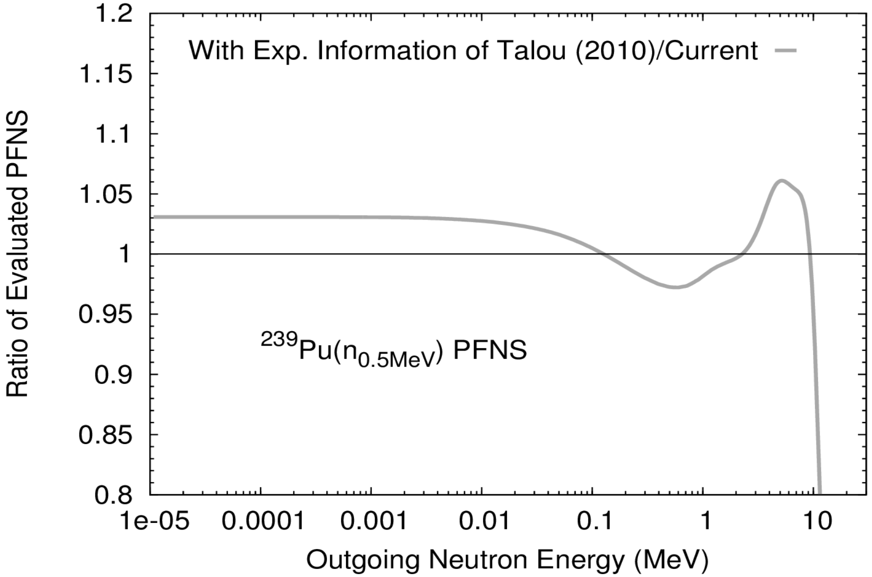
Chi Nu project at LANSCE will provide new data.

Invited Nucl. Data Sheets contribution with R.C. Haight, T.N. Taddeucci, H.Y. Lee, M.C. White, M.E. Rising, in preparation.

The ^{239}Pu PFNS Evaluation: Experimental Data and Uncertainties

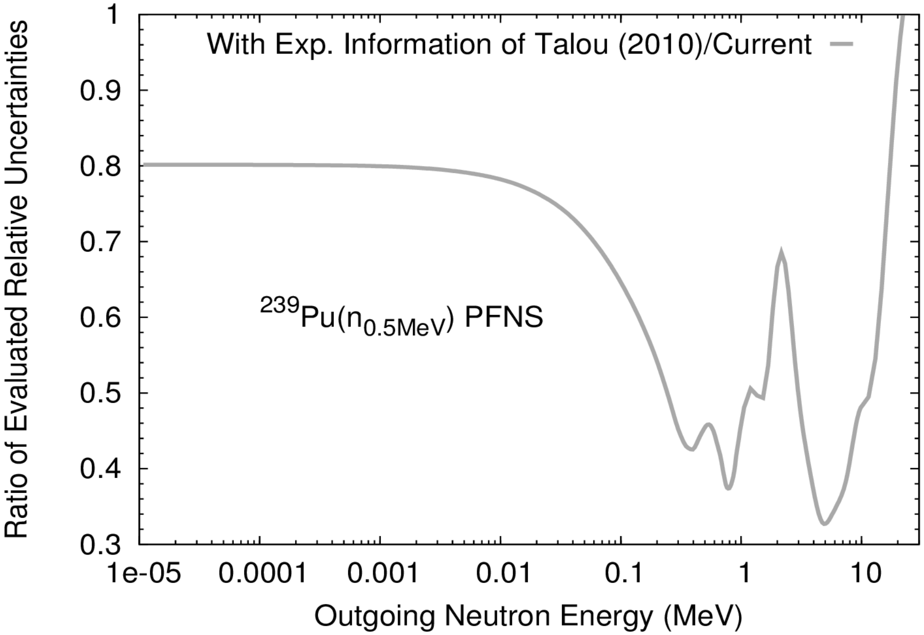
Does an improved exp. UQ matter?

Using the *improved experimental UQ*, leads to *significant changes in evaluated uncertainties.*

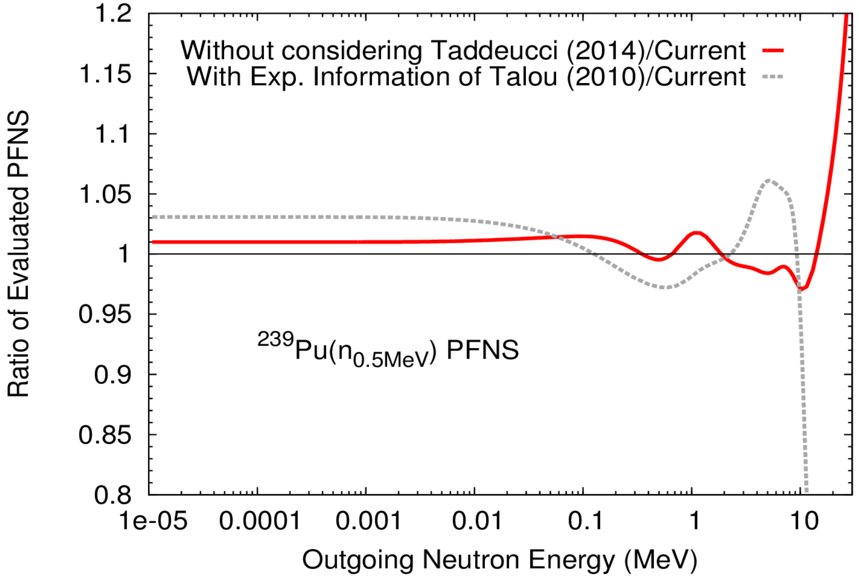


k_{eff} uncertainty reduced by ~67% for Jezebel.

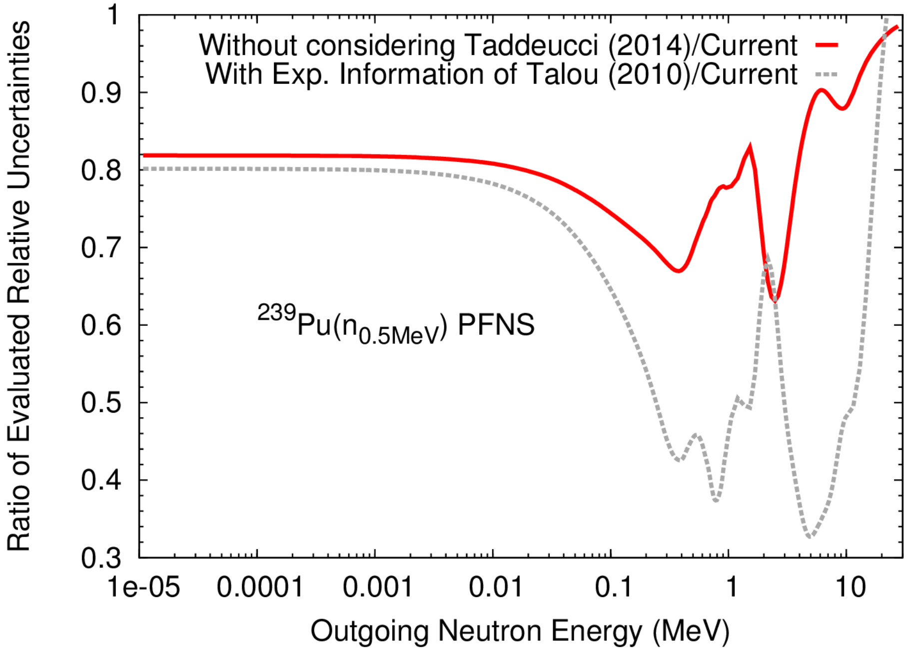
D. Neudecker, P. Talou, T. Kawano, Transactions of the American Nuclear Society **111**, 1415 (2014)



Additional unc. estimated using *MCNP studies of Taddeucci et al. influence the eval. PFNS and unc.*

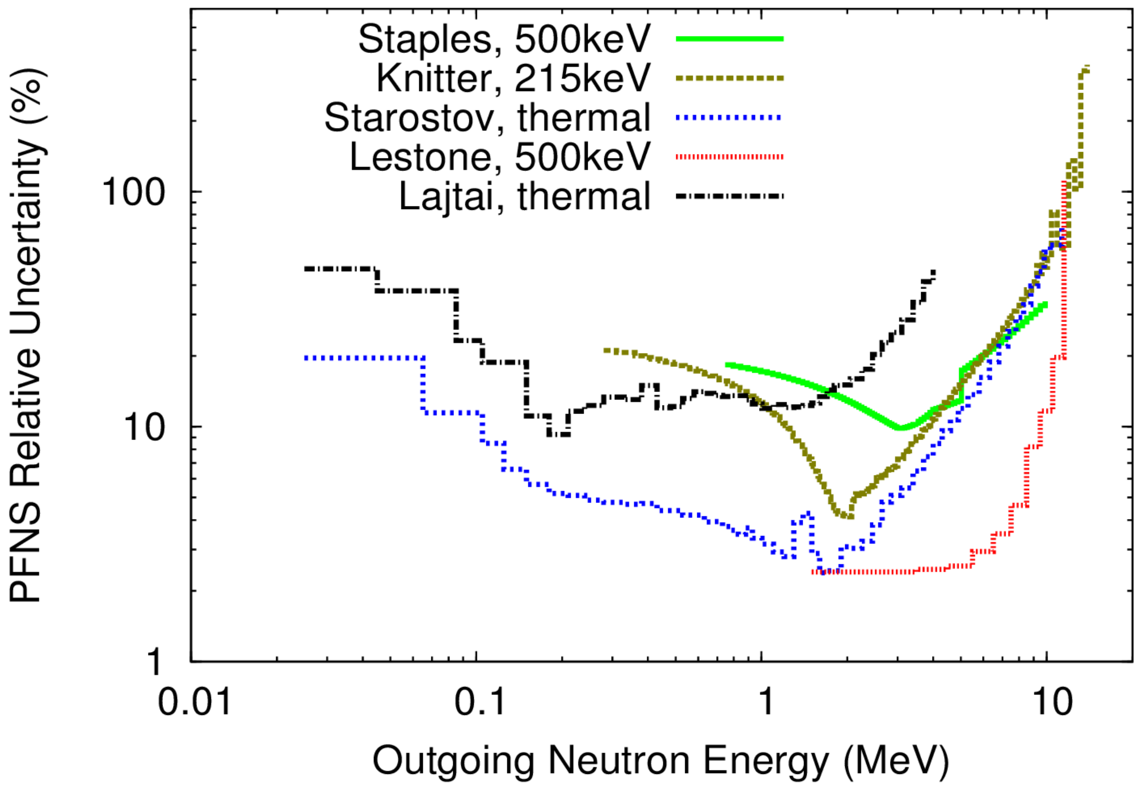


k_{eff} uncertainty reduced by ~20% for Jezebel.



D. Neudecker, P. Talou, T. Kawano, Transactions of the American Nuclear Society **111**, 1415 (2014)

New experiments for E_{inc} < 500 keV impact the evaluation only with similar unc. to Starostov data.



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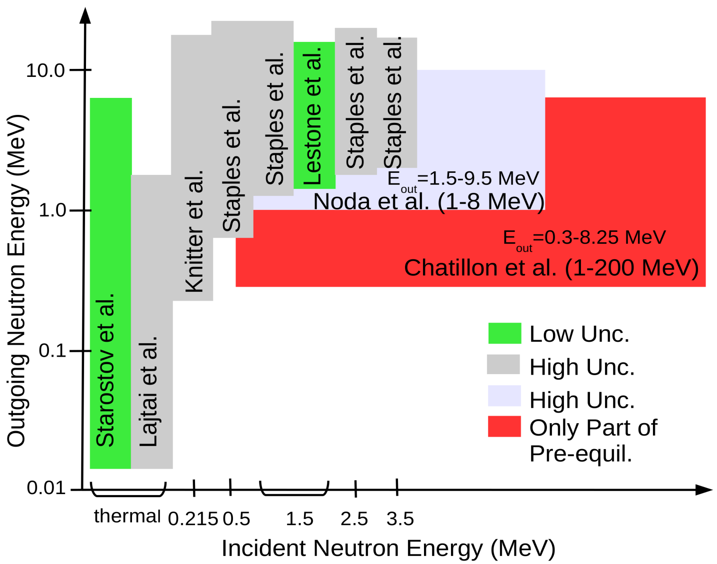
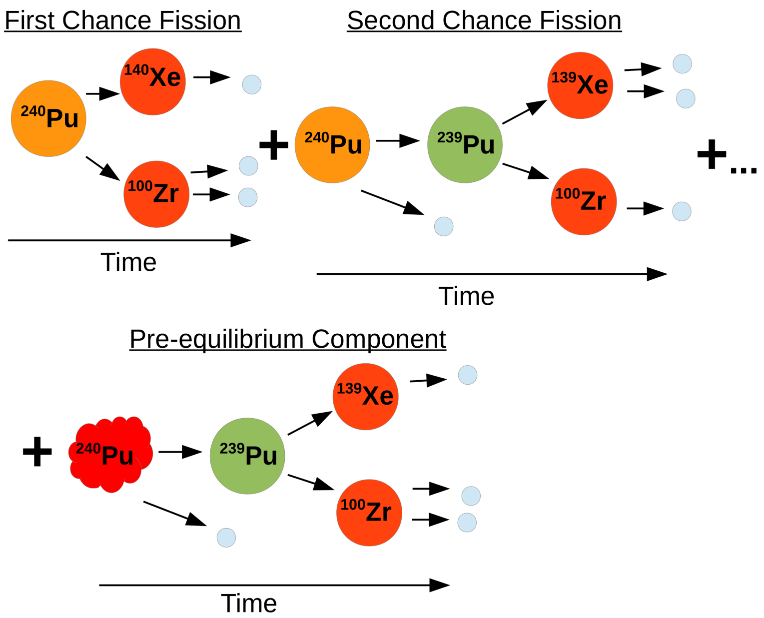
The ^{239}Pu PFNS Evaluation: Model Information



Why do we need model information and why extend the model?

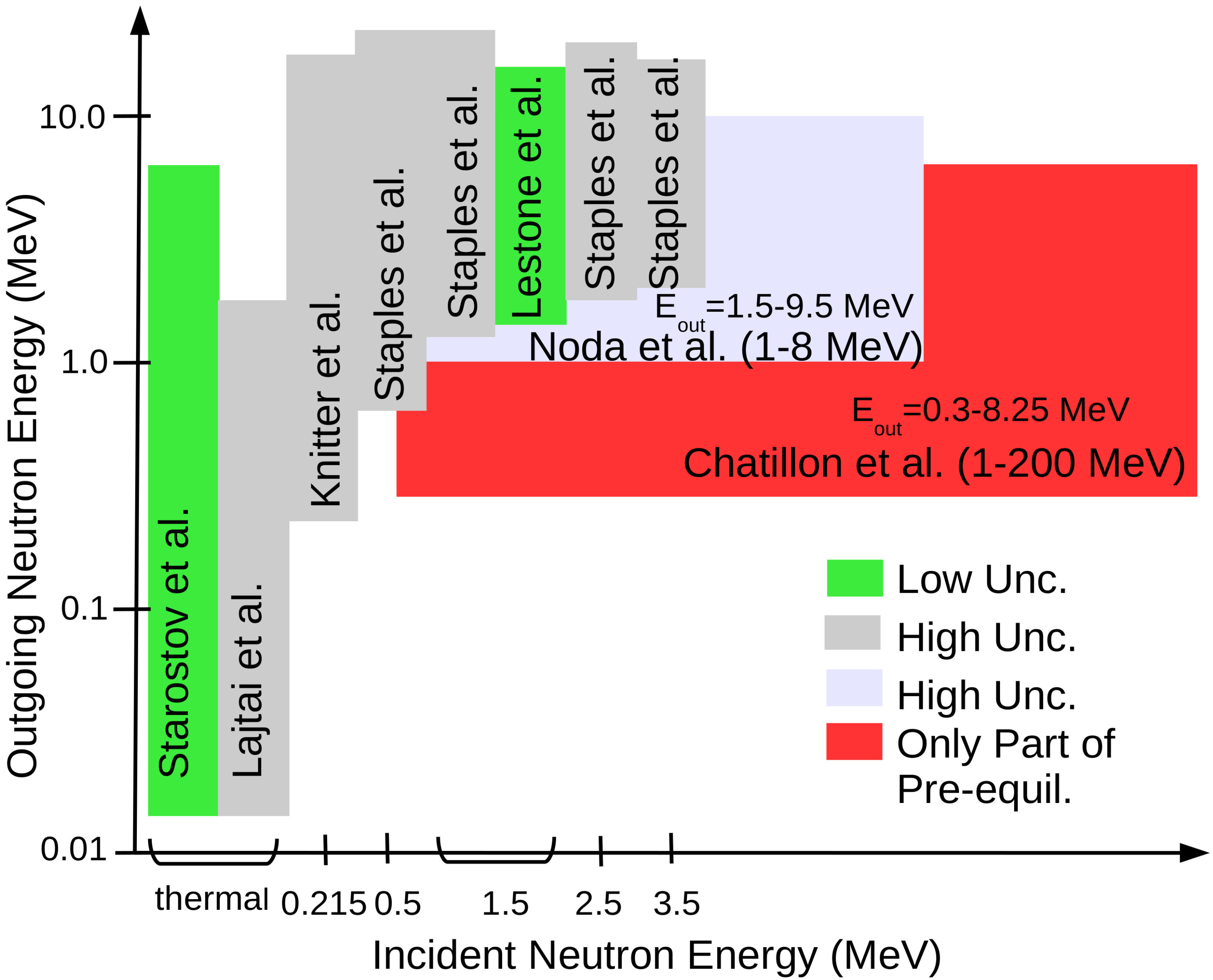


Getting improved physics for E_{inc} = thermal – 30 MeV?

The ^{239}Pu PFNS Evaluation: Model Information

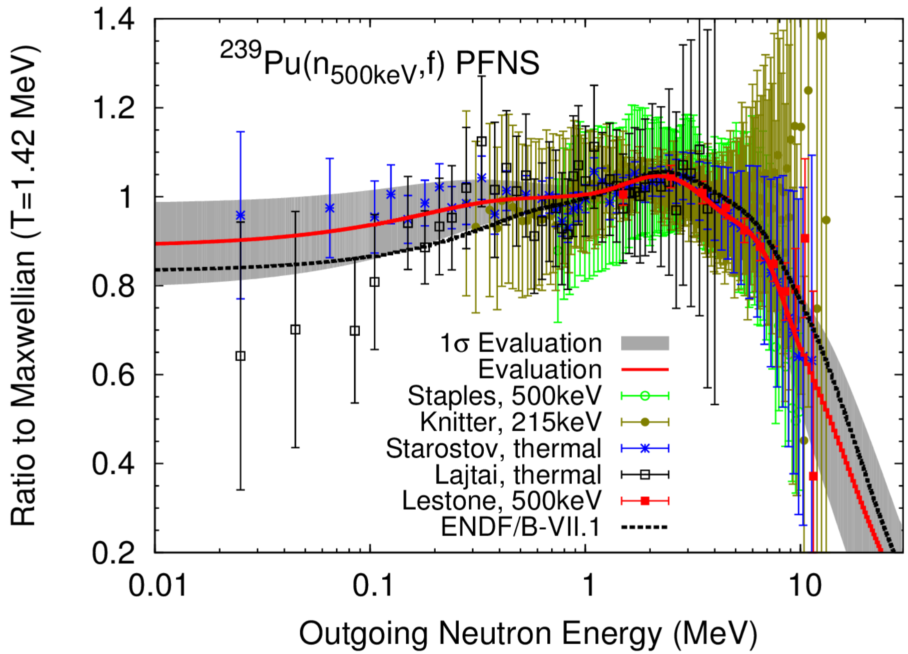
Why do we need model information and why extend the model?

Model information needed due to scarce exp. information.

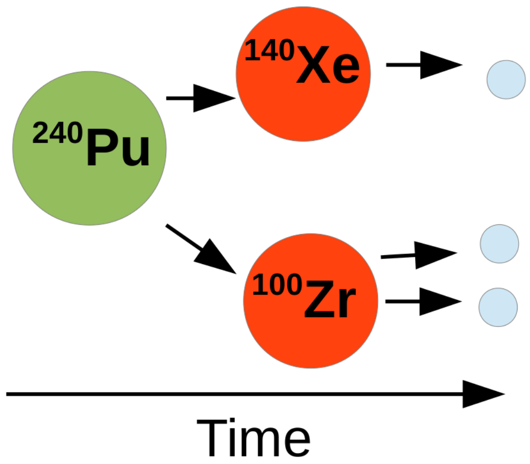


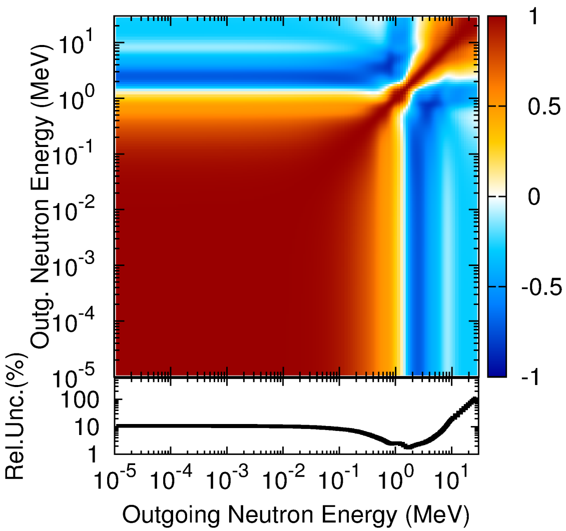
~20% of neutrons predicted below 700 keV

At E_{inc} = 500 keV, we deal with enough exp. data and first chance fission physics ...



First Chance Fission





D. Neudecker, P. Talou, T. Kawano, D.L. Smith, R. Capote, M.E. Rising, A.C. Kahler NIMA **791**, 80 (2015).

… but there is still the problem of low evaluated uncertainties ...

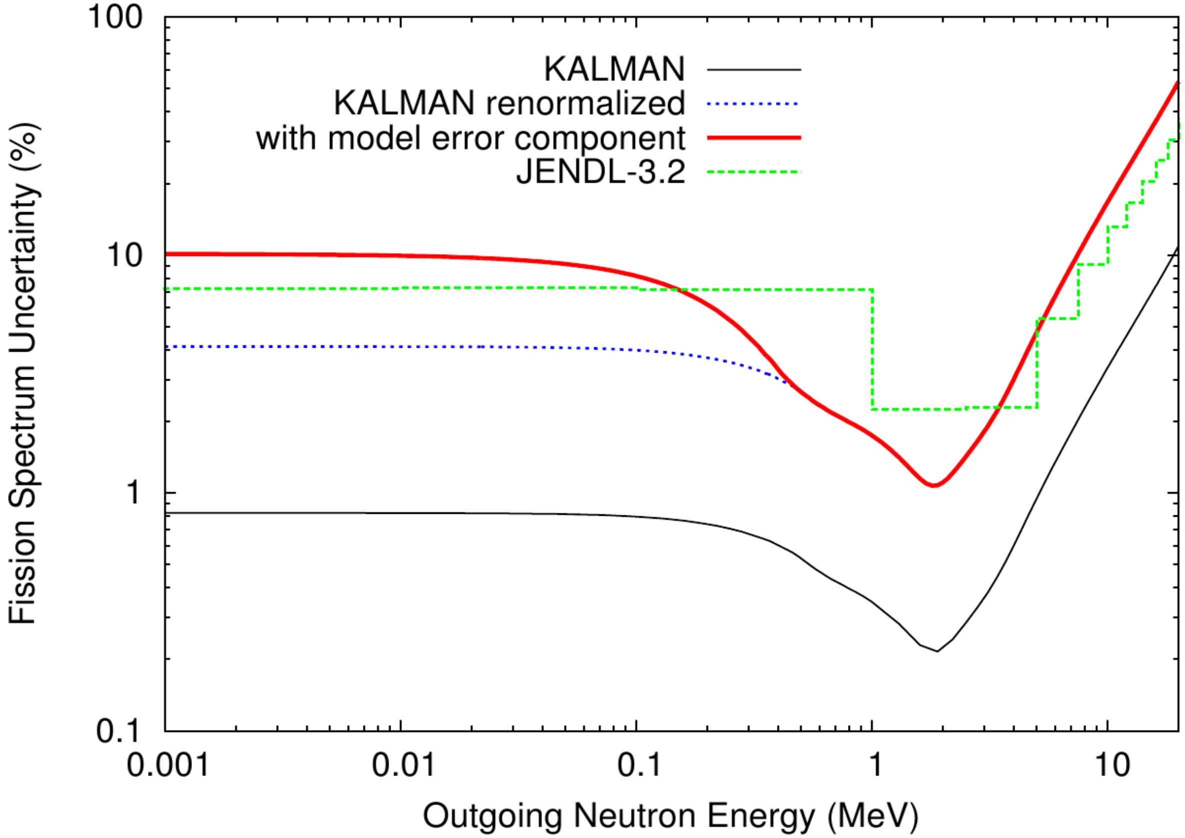
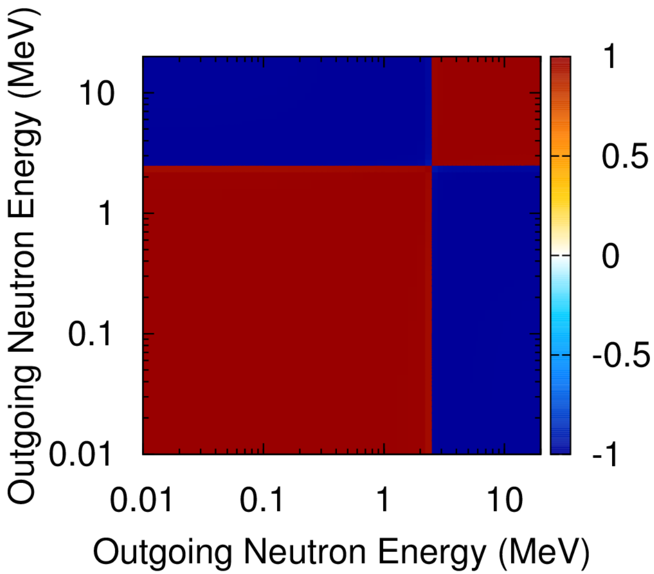


FIGURE 4. Calculated standard deviations for the evaluated PFNS of n(0.5 MeV)+^{239}Pu. See text for details.

Taken from P. Talou et al. LA-UR-19-00646, published in NSE **166, 254** (2010).

… which is caused by the normalization condition on the PFNS & cov. and strong model correlations.



Talou (2010)

- Normalization condition reduces unc.:

$$\sum_i \varphi\left(E^i_{out}\right)\Delta E^i_{out}=\sum_i \Phi\left(E^i_{out}\right)=1$$

$$\frac{\sum_j Cov\left(\varphi\left(E^i_{out}\right),\varphi\left(E^j_{out}\right)\right)}{\varphi\left(E^i_{out}\right)}<10^{-5}$$

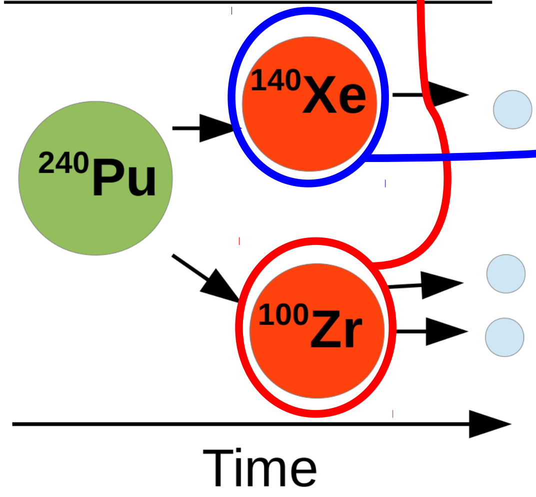
- Strong model correlations questionable → include ***more physically justifiable model parameters***

D. Neudecker, R. Capote, D.L. Smith, T. Burr, P. Talou, NSE **179**, 381 (2015).

The LAM PFNS are a weighted sum of average light and heavy fission fragment PFNS.

$$\chi_1(E)=\frac{\overline{\nu}_{1L}\chi_{1L}(E,T_{mL},a_L,b,s,...)+\overline{\nu}_{1H}\chi_{1H}(E,T_{mH},a_H,b,s,..)}{\overline{\nu}_{1L}+\overline{\nu}_{1H}}$$

First Chance Fission



The **Los Alamos model** (D.G. Madland et al., Nucl. Science Eng. **81**, 213 (1982)) as included in the **CoH code** (by T. Kawano) is used.

Extended the LAM by considering neutron multiplicity of light and heavy fragment.

$$\chi_1(E) = \frac{\overline{\nu_{1L}}\chi_{1L}(E, T_{mL}, a_L, b, s, \ldots) + \overline{\nu_{1H}}\chi_{1H}(E, T_{mH}, a_H, b, s, \ldots)}{\overline{\nu_{1L}} + \overline{\nu_{1H}}}$$

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

Maxwellian shape integrated over temperature distribution.

$\overline{\nu_{1L}} \neq \overline{\nu_{1H}}$ and $T_{mL} \neq T_{mH}$ (e.g., T. Ohsawa et al., Nucl. Phys. A **665**, 3 (2000).)

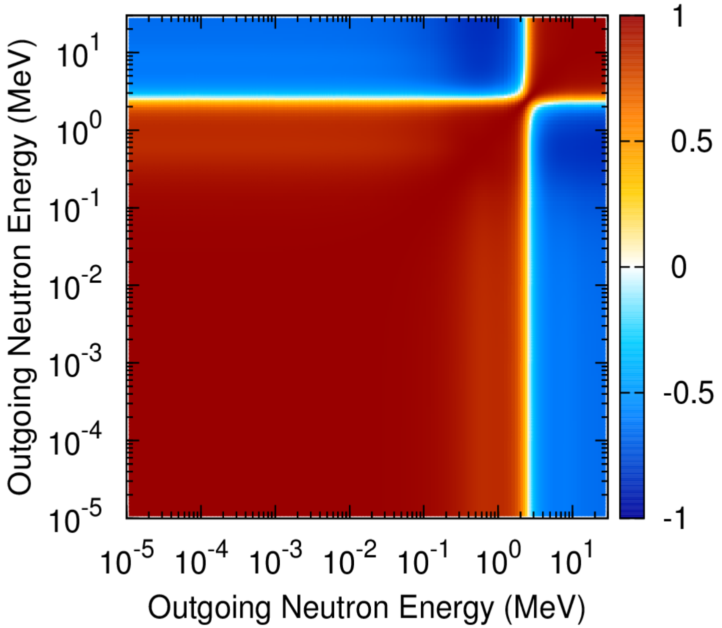
Extended the LAM by new temperature distribution and anisotropy.

$$N(E) = \frac{1}{2\sqrt{E_f}T_m^2}\boxed{\frac{1}{1+b/3}}\int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} d\varepsilon\sigma_c(\varepsilon)\sqrt{\varepsilon}\boxed{\left(1+b\frac{(E-\varepsilon-E_f)^2}{4\varepsilon E_f}\right)}\boxed{\int_0^{T_m} dTk(T)T\exp(-\varepsilon/T)}$$

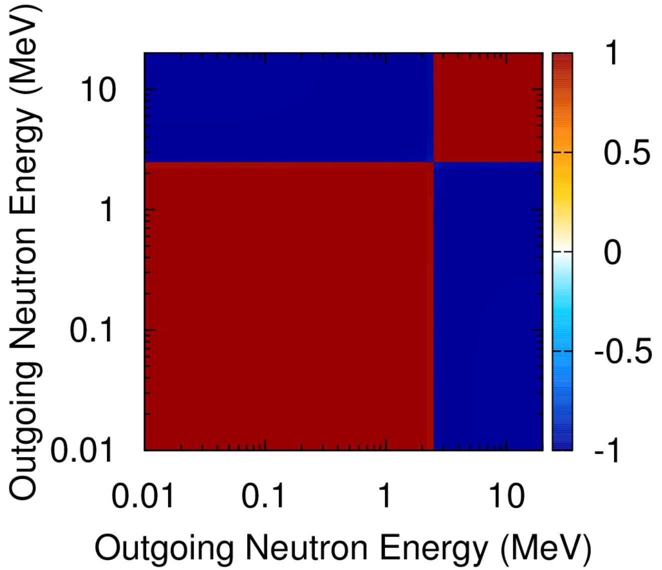
- With ***b***, an ***anisotropy in the neutron emission*** in the cms frame is considered effectively (J. Terrell, Phys. Rev. **113**, 527 (1959), already implemented in eval. of M.E. Rising et al., NSE **175**, 81 (2013).)

- Instead of a triangular ***temperature distribution***, one by F.-J. Hambsch et al., ANE **32**, 1032 (2005) is considered (with parameter ***s***).

Model correlations are weakened by including new parameters.

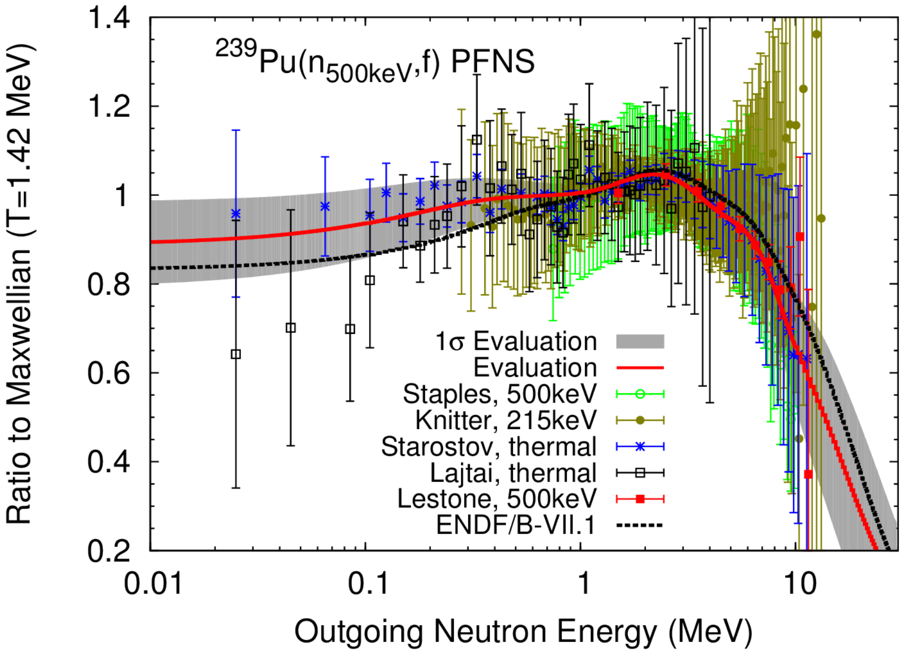


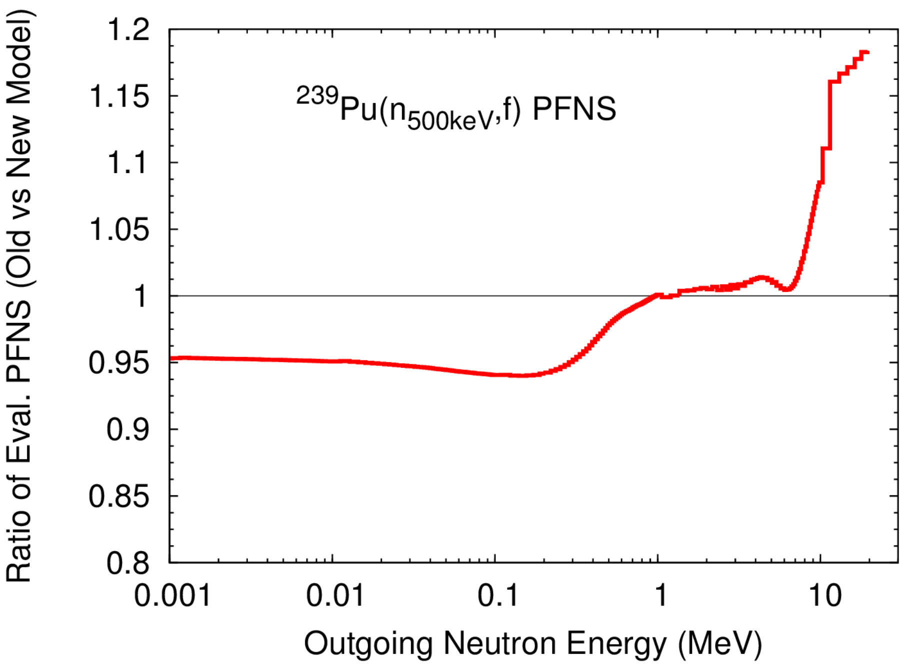
This Work



Talou (2010)

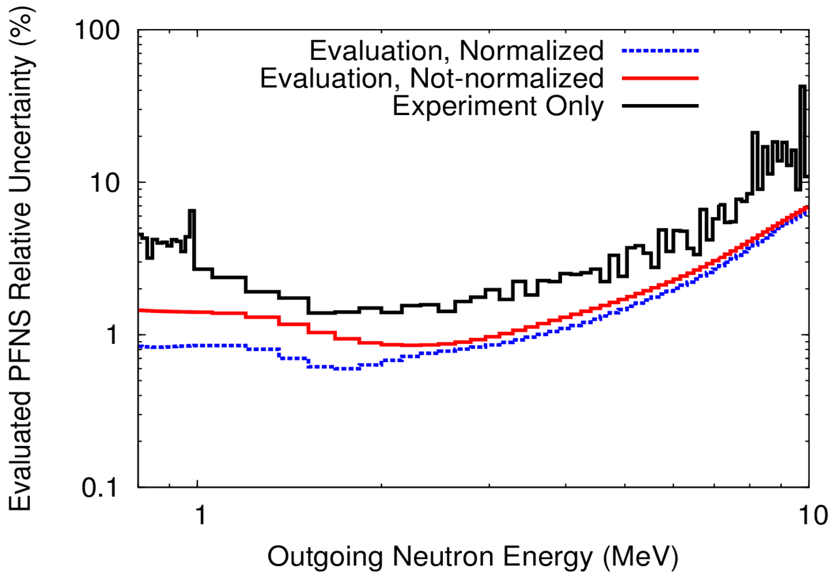
The extension of the LAM has a noticeable impact on the evaluated PFNS.



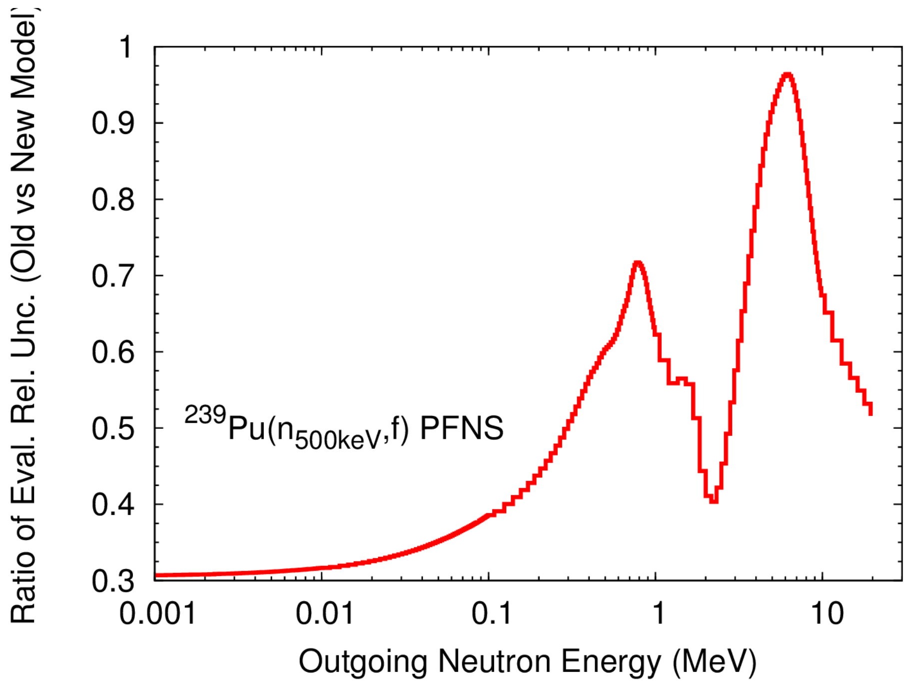


D. Neudecker et al., NIMA **791**, 80 (2015).

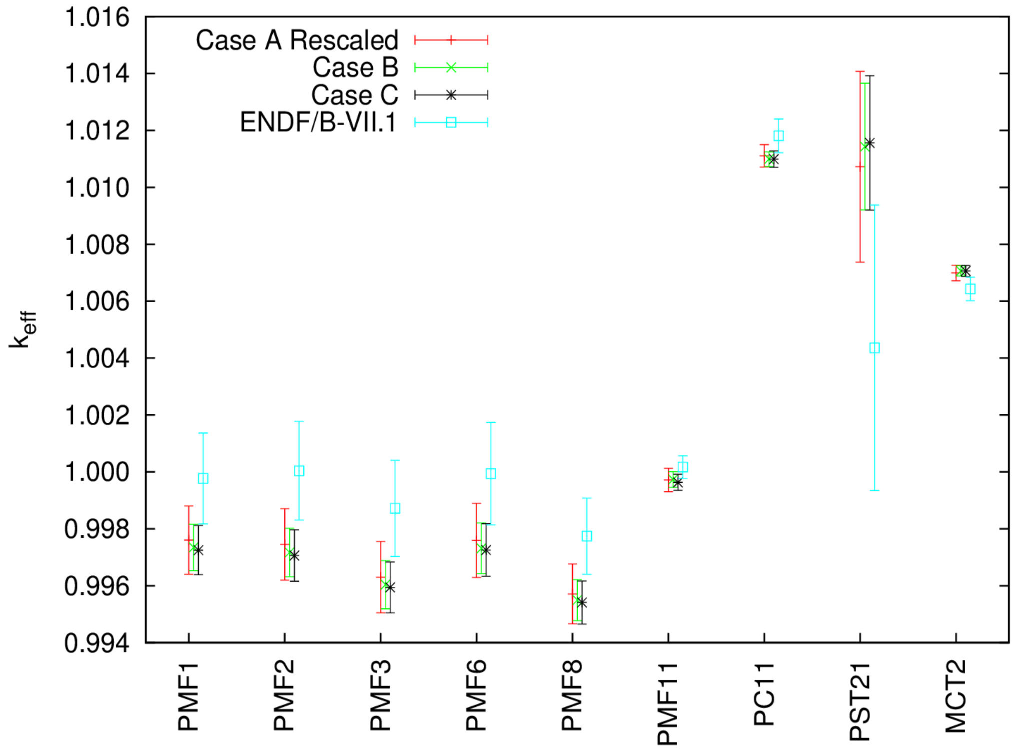
Using the extended LAM leads to more reasonable eval. unc. compared to exp. input.



Still not perfect, approaches to model defects in D. Neudecker et al., NIMA **791**, 80 (2015).



The new evaluation changes the benchmarks.

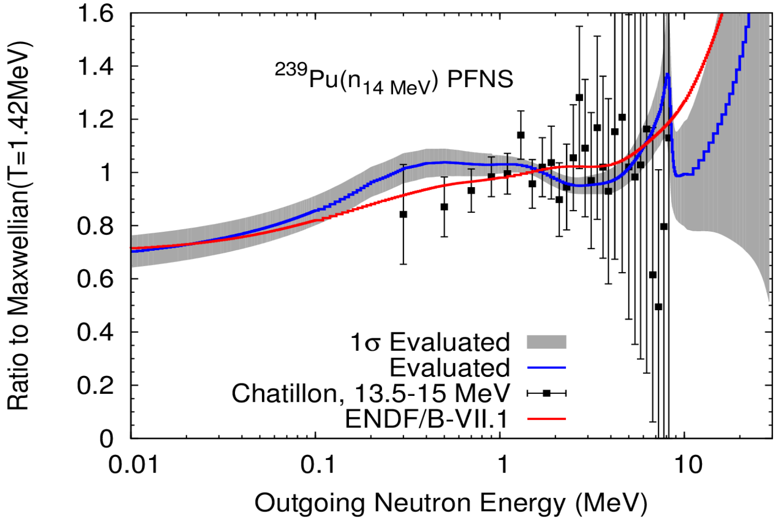


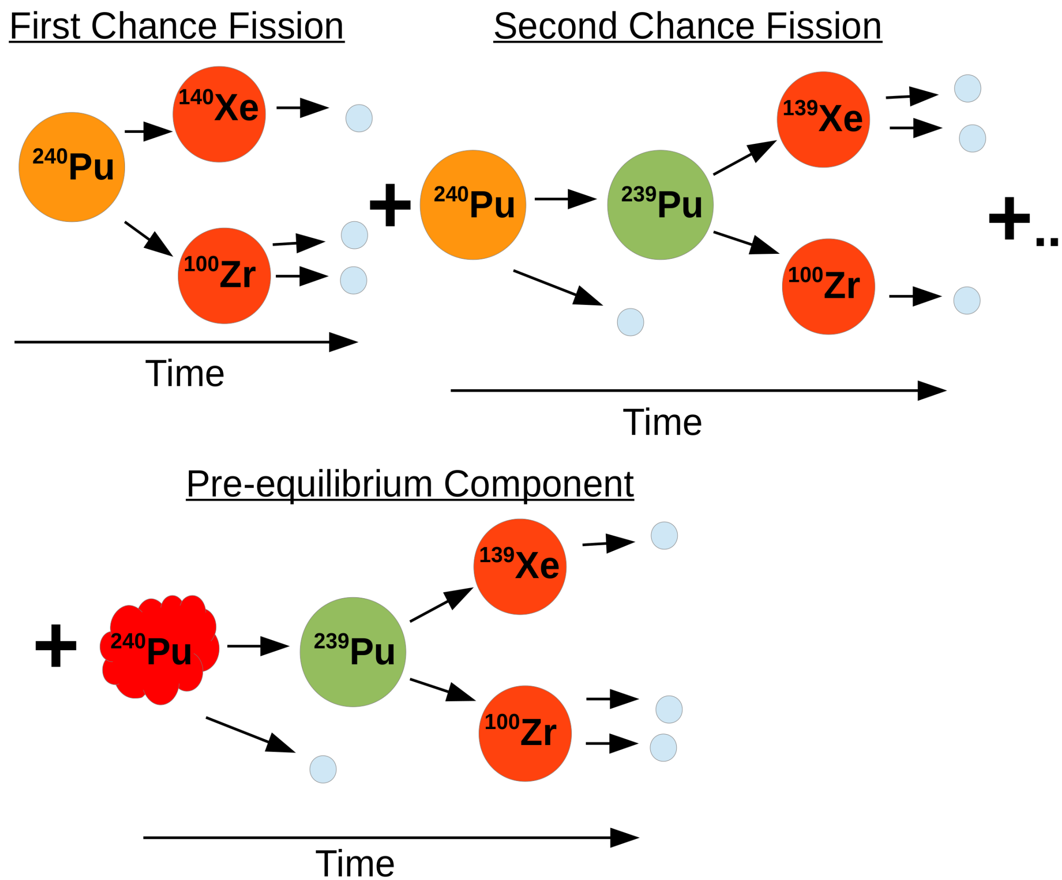
D. Neudecker et al., NIMA **791**, 80 (2015).

The ^{239}Pu PFNS Evaluation: Model Information

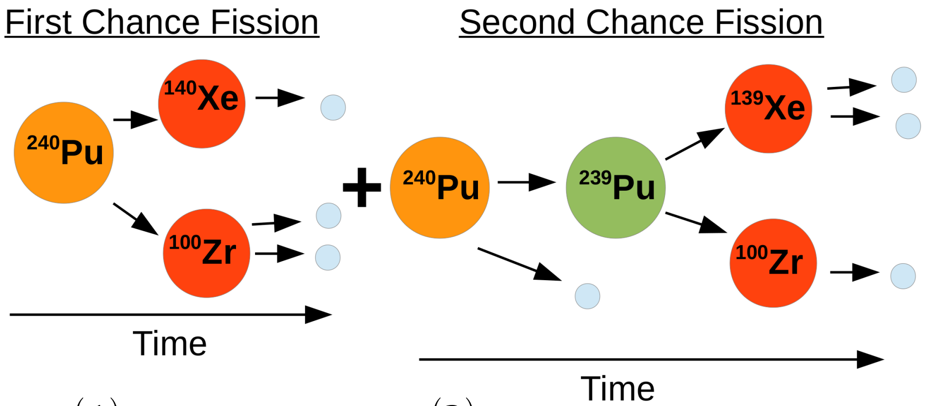
Getting improved physics for E_{inc} = thermal – 30 MeV?

At higher E_{inc}, we deal with more physics processes and scarce exp. info.





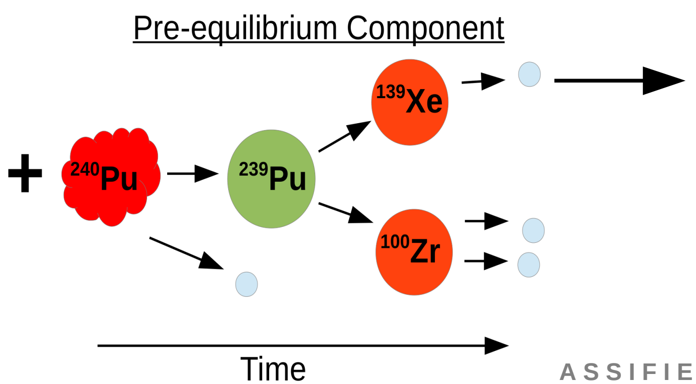
These physics processes are considered in our model description.



The **LAM** is used for **compound nucleus processes.**

$$\chi(E) \propto p_f^{(1)} \overline{\nu}_1 \chi_1(E) + p_f^{(2)} [\phi_1(E) + \overline{\nu}_2 \chi_2(E)]$$

$$+ p_f^{(3)} [\phi_1(E) + \phi_2(E) + \overline{\nu}_3 \chi_3(E)] + \ldots$$



ASSIFIED

The **exciton model** in CoH is used for the **pre-equilibrium component.**

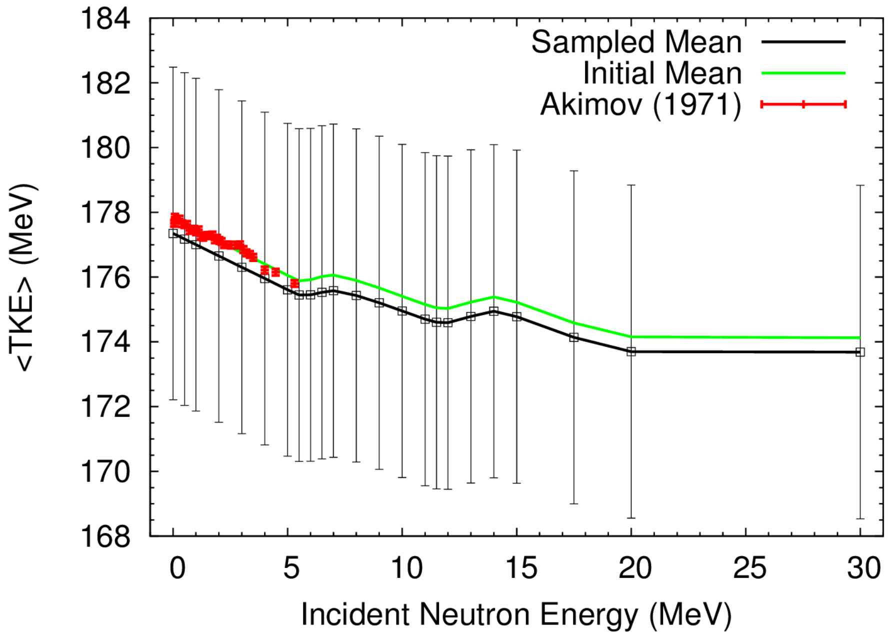
We also consider an improved parametrization of model parameters.

- ***E_{inc}-dependent parametrization of <TKE> and <E_r>*** of Lestone (Lestone et al., NDS **118**, 208 (2014).) and Madland

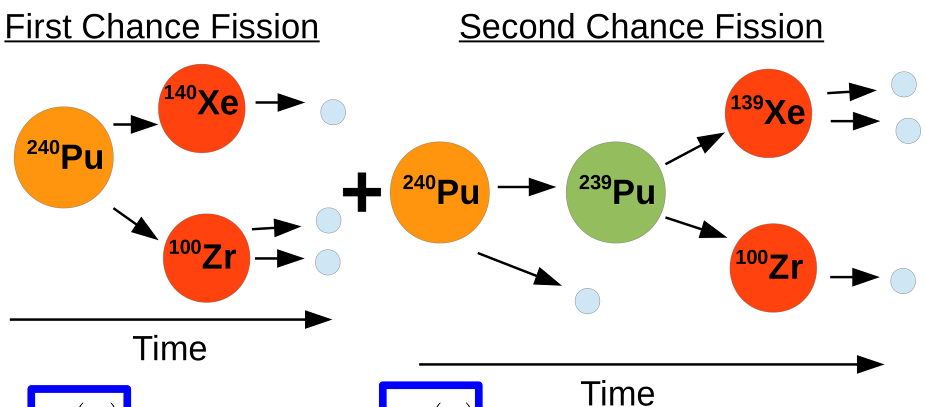
$$N(E) = \frac{1}{2\sqrt{E_f}T_m^2}\int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} d\varepsilon \sigma_c(\varepsilon)\sqrt{\varepsilon} \times \int_0^{T_m} dT k(T) T \exp(-\varepsilon/T)$$

$$T_{m,x} = \sqrt{\langle E^* \rangle / \langle a_x \rangle}$$

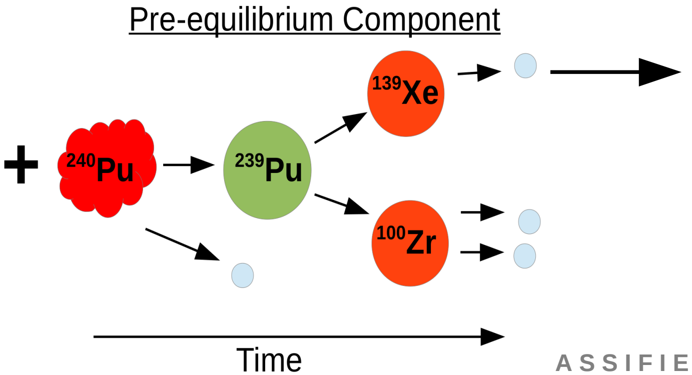
$$\langle E^* \rangle = \langle E_r \rangle + E_{\mathrm{inc}} + B_n - \langle TKE \rangle$$



Fission probabilities are calculated via fission barrier parameters.



$$\chi(E) \propto \boxed{p_f^{(1)}}\,\overline{\nu_1}\,\chi_1(E) + \boxed{p_f^{(2)}}\left[\phi_1(E) + \overline{\nu_2}\,\chi_2(E)\right] + \boxed{p_f^{(3)}}\left[\phi_1(E) + \phi_2(E) + \overline{\nu_3}\,\chi_3(E)\right] + \ldots$$



Fission barrier parameters fitted to reproduce ENDF/B-VII.0 fission probabilities.

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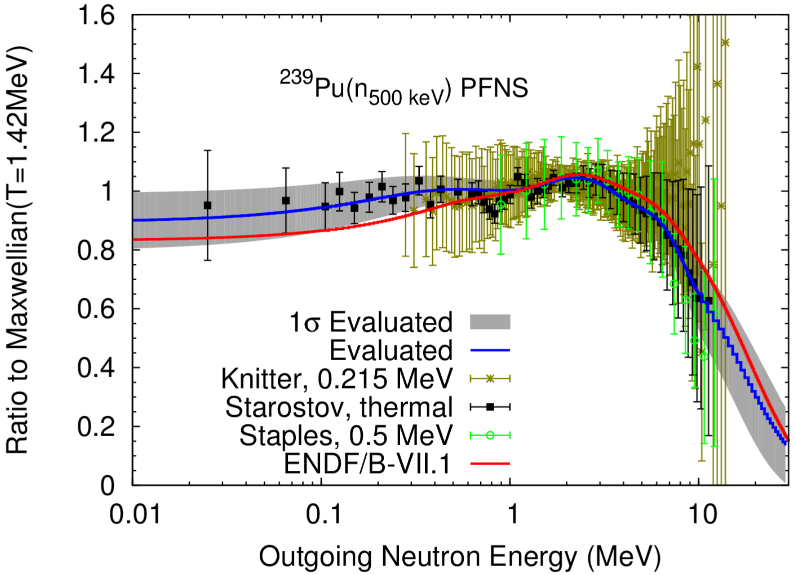
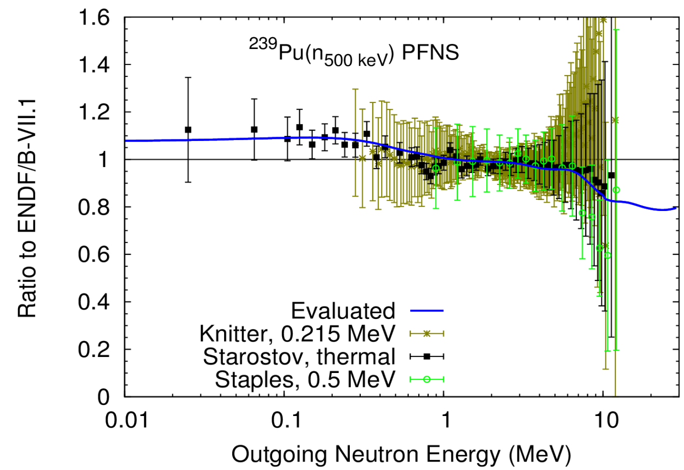
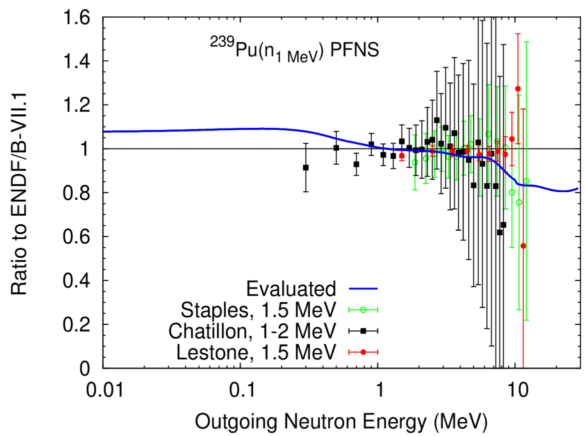
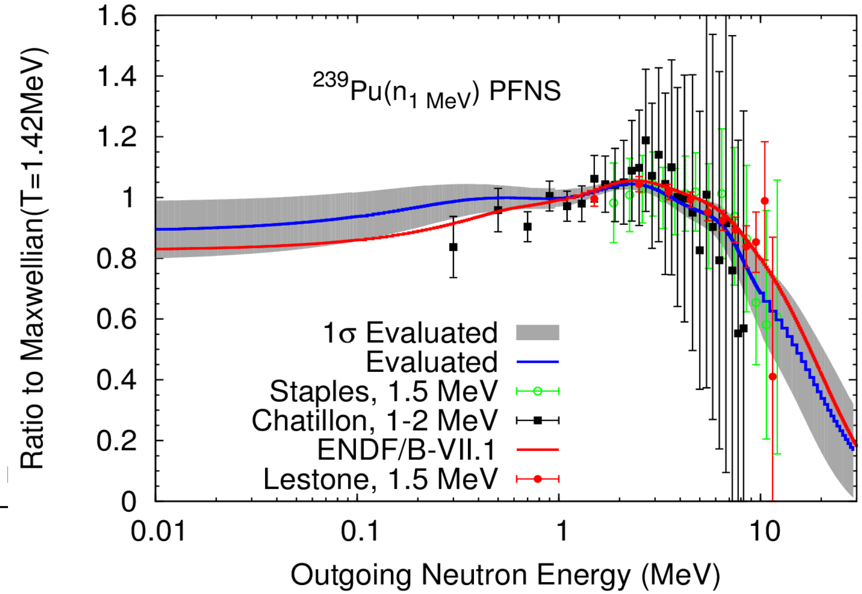
At E_{inc} = 500 keV, we see similar tendencies compared to the test-case evaluation.

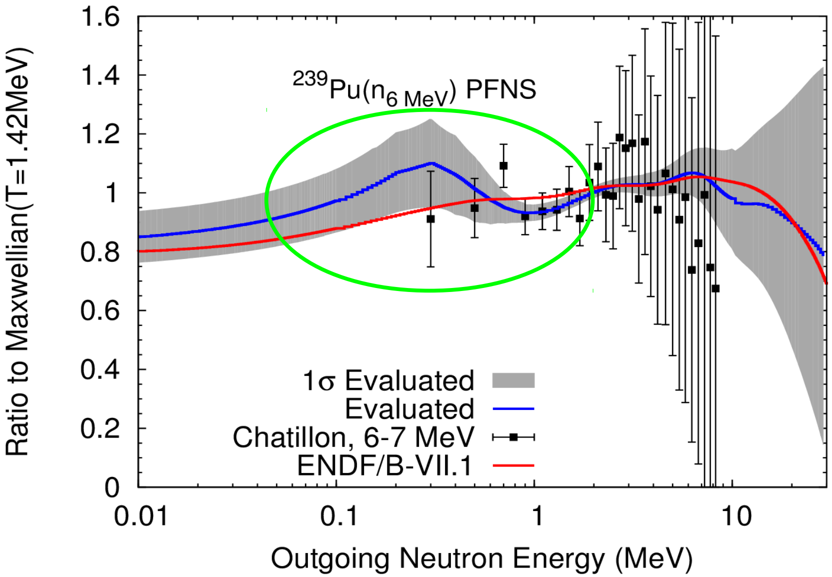


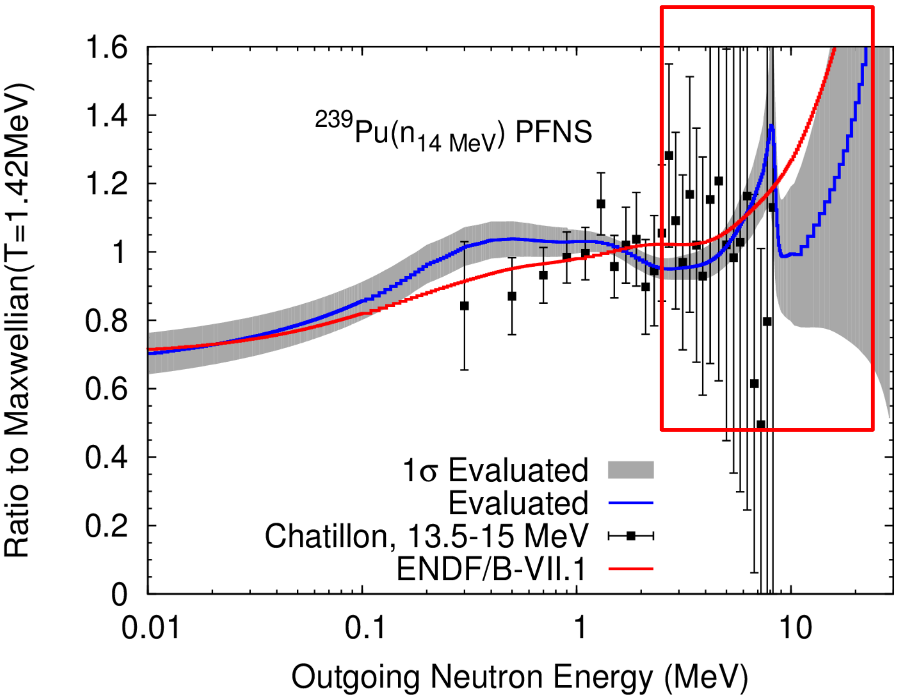


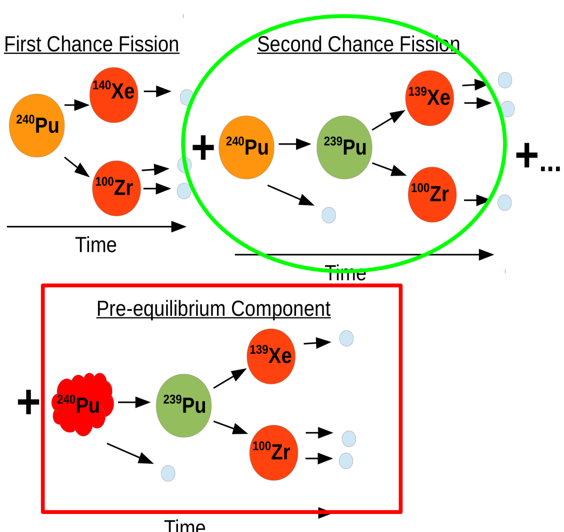




We see differences compared to ENDF/B-VII.1 due to additional physics processes.







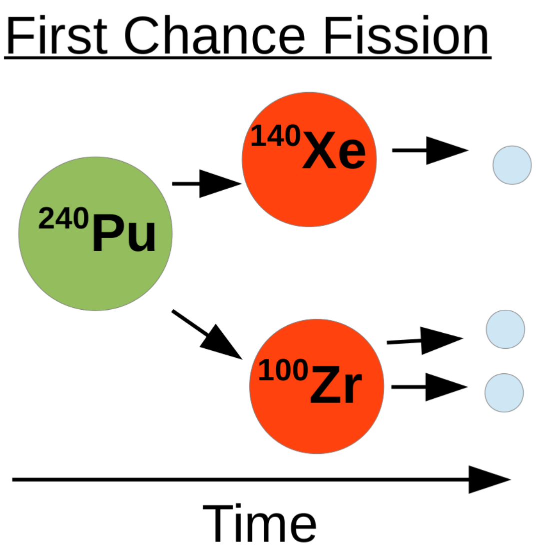
The ^{239}Pu PFNS Evaluation: Model Information

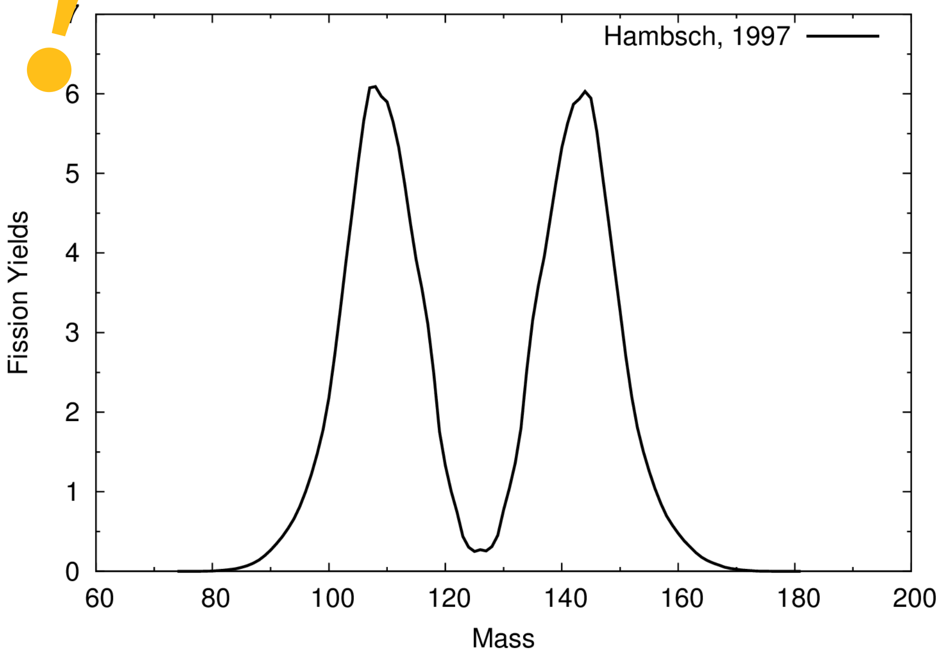
Getting improved physics ????

Future activities: Use a model which describes the fission process in more detail.

LAM averages over few fission fragment pairs, but many more are emitted.

?!



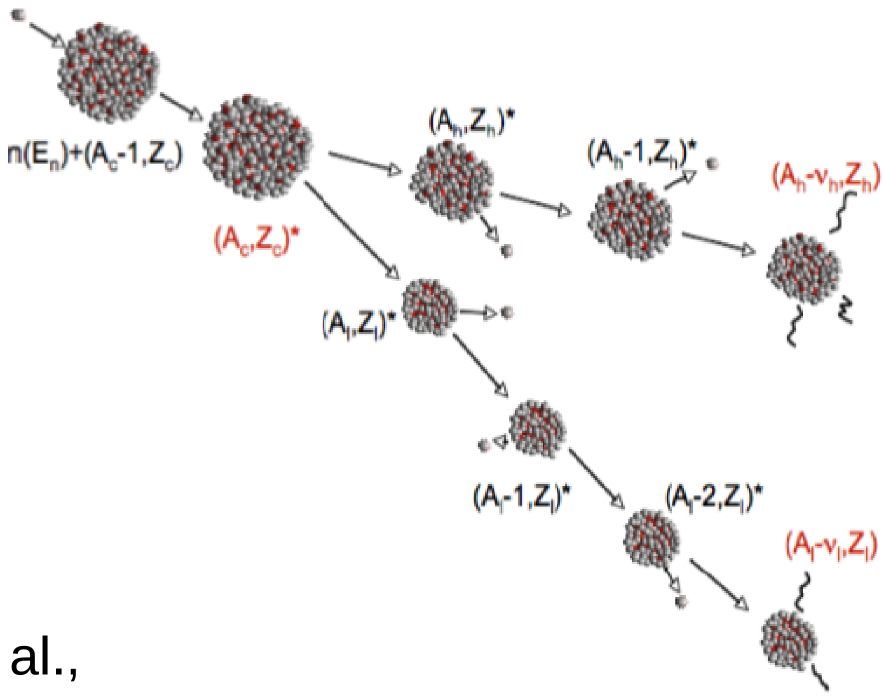


Future activities: Use a model which describes the fission process in more detail.

MCHF code (Talou, T. Kawano and I. Stetcu) follows each decay step.

Provide **predictions of several fission quantities** (PFNS, multiplicity, γ-spectrum, etc.) and several isotopes

→ **MORE (measurable) INPUT QUANTITIES NEEDED.**



Recent paper: I. Stetcu et al., PRC **90**, 024617 (2014).

Thanks to P. Talou for this figure.

Summary ...

- Nuclear data evaluation combines theoretical and experimental information for nuclear data applications.

- We made an ***improved uncertainty estimate of experimental ^{239}Pu PFNS*** and ***extended the Los Alamos*** model to get more reasonable evaluated uncertainties for E_{inc} = 500 keV.

- The ***^{239}Pu PFNS* evaluation was extended up to E_{inc} = of 30 MeV**, including new experimental data and missing physics processes

... and to-do

- Include new experimental data once they are available.

- Use a **model taking into account the many fragmentation pairs occurring in the fission process** and verify PFNS data by means of cross-correlation to other fission quantities.

- Is our model and experimental data really normally distributed? Do we bias our results using Generalized Least Squares?

Thanks to my current collaborators on this project …

P. Talou, T. Kawano, A.C. Kahler (T-2)
M.C. White, M.E. Rising, J.P. Lestone, D. Vaughan (X)
Chi Nu: especially R.C. Haight, T.N. Taddeucci, H.Y. Lee (P-27)
F. Tovesson (P-27), T. Burr (CCS-6), R. Capote (IAEA), D.L. Smith (ANL)

And: Thank you for your attention!

Literature related to this work:

+) Neudecker, Talou, Kawano, Smith, Capote, Rising, Kahler, NIMA **791**, 80 (2015).

+) Talou et al., NSE **166,** 254 (2010).

+) Rising et al., NSE **175**, 81 (2013).

+) Neudecker, Capote, Smith, Burr, Talou, NSE **179**, 381 (2015).

+) Neudecker, Talou, Kawano, Transactions of the American Nuclear Society **111**, 1415 (2014).

+) Taddeucci et al., Nuclear Data Sheets **123**, 135 (2015).

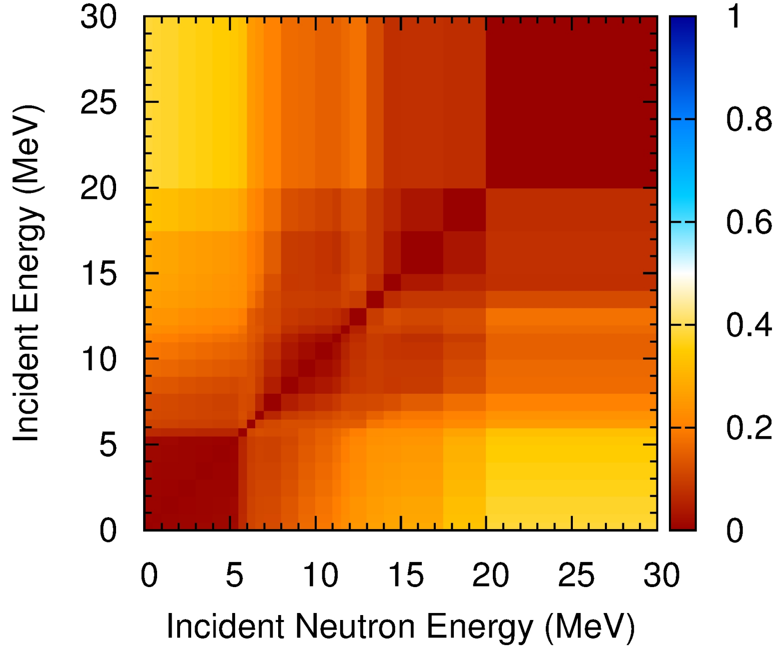
+) Madland et al., NSE **81**, 213 (1982).

+) Lestone et al., NDS **118**, 208 (2014).

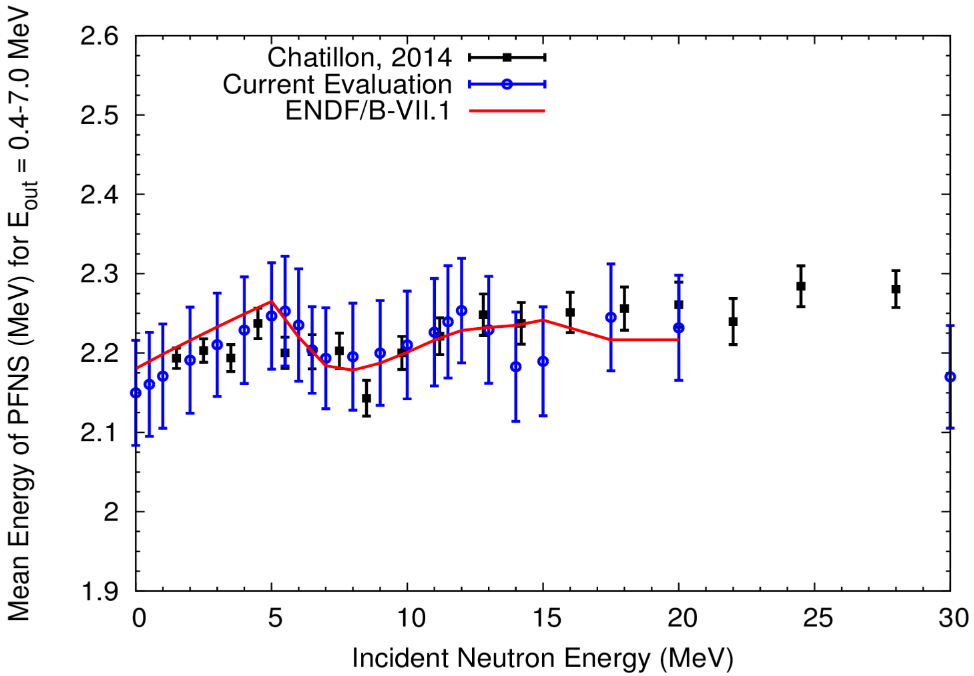
+) Neudecker, Capote, Leeb, NIMA **723**, 163 (2013).

We also provide covariances for all E_{inc} of eval. PFNS and mean energies.

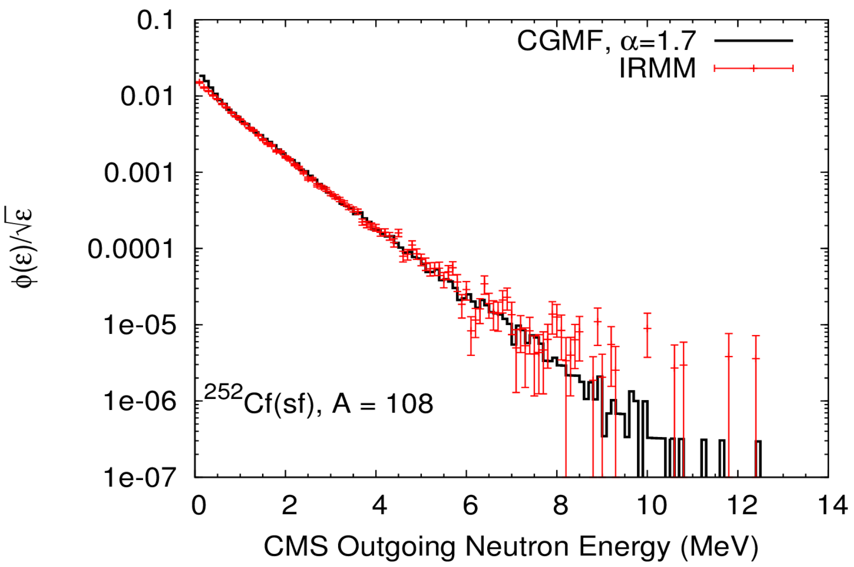
Mean of difference between correlations of different E_{inc}



Correlations between different E_{inc} are also provided.



One step: Improving the model by comparison to additional experimental data.



PFNS for certain mass ranges can be used to improve CGMF input parameters.