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Title: Modeling and evaluating 239Pu and 235U PFNS and average prompt-neutron multiplicity

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Los Alamos NATIONAL LABORATORY

Modeling and evaluating ^{239}Pu and ^{235}U PFNS and average prompt-neutron multiplicity

Amy Lovell & Denise Neudecker

NCSP TPR, 2/16/2022

LA-UR-22-xxxxx

This work shows progress towards fulfilling NCSP milestones of LANL ND1 (Nuclear Data Evaluation and Testing).

Thanks to: M.B. Chadwick, M. Devlin, I. Stetcu, K. Kelly, R.C. Little, T. Kawano, P. Marini, L. Snyder, J. Taieb, P. Talou.

FY21-22 milestones:

- ^{239}Pu, ^{235}U: "Update fission cross section based on TPC results (from ^{239}Pu/^{235}U ratio data)" (DUE FY21 Q4),

- ^{235}U, ^{239}Pu: "Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons" (DUE FY22 Q4),

- ^{235}U: "Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu" (DUE FY22 Q2),

- And ^{235}U: "Develop consistent evaluation of fission yields, neutron multiplicity, and spectra from thermal to 20 MeV" (DUE FY22 Q4).

FY21-22 milestones:

- ^{239}Pu, ^{235}U: "Update fission cross section based on TPC results (from ^{239}Pu/^{235}U ratio data)" (DUE FY21 Q4),
- ^{235}U, ^{239}Pu: "Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons" (DUE FY22 Q4),
- ^{235}U: "Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu" (DUE FY22 Q2),
- And ^{235}U: "Develop consistent evaluation of fission yields, neutron multiplicity, and spectra from thermal to 20 MeV" (DUE FY22 Q4)

Two of the milestones are reached with the LANL-developed Hauser-Feshbach Fission Fragment Decay Codes CGMF (Monte Carlo) and BeoH (deterministic)

Modeling

- CGMF and BeoH, LANL's Monte Carlo and deterministic fission fragment decay codes
- Challenges in the PFNS
- Consistency between neutron multiplicity and fission product yields

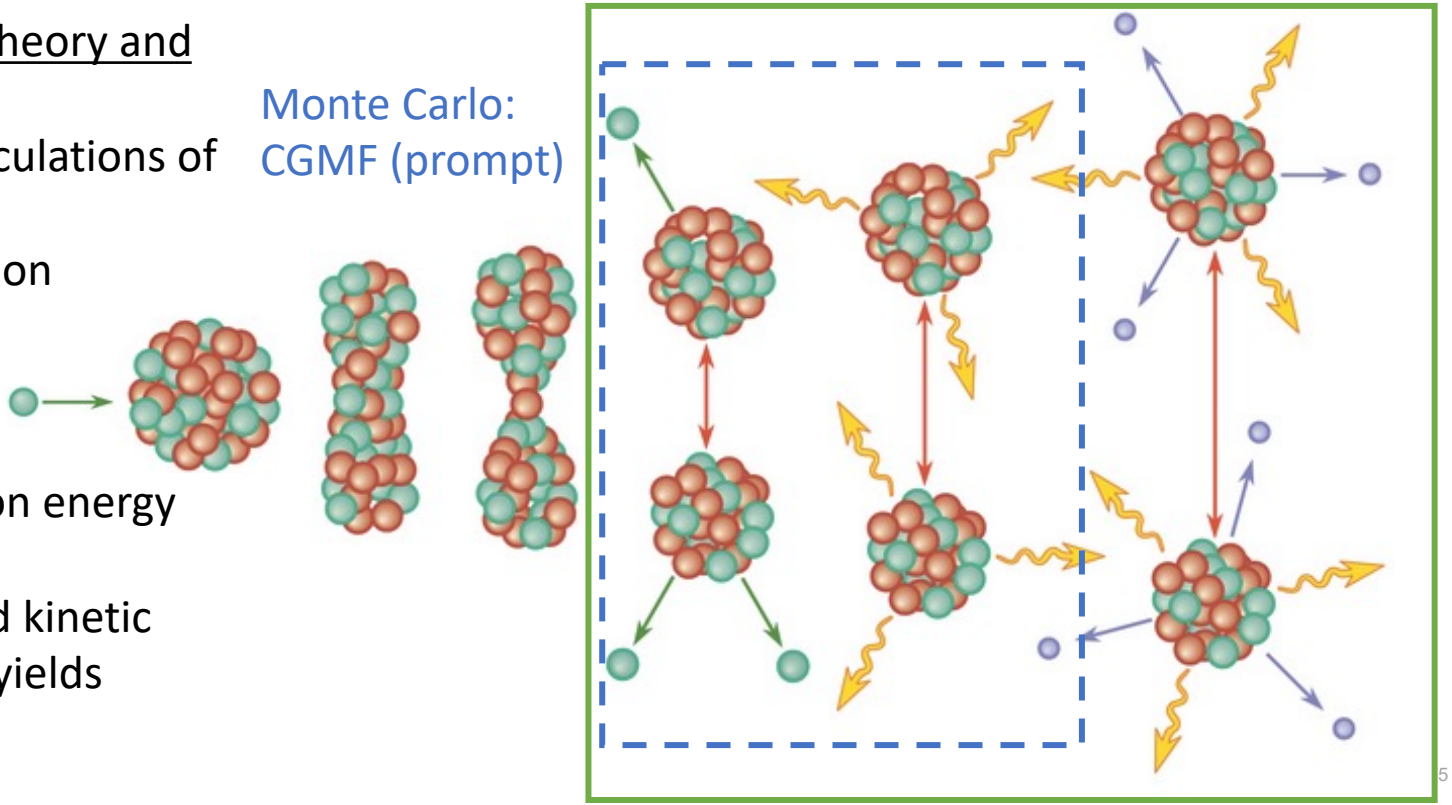
Monte Carlo and deterministic models at LANL

Deterministic: BeoH (prompt and delayed)

<u>Input needed from theory and experiment:</u>

- First-principle calculations of fission yields
- Multi-chance fission probabilities

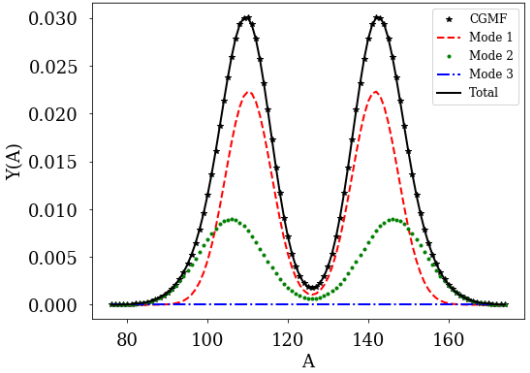
Monte Carlo:
CGMF (prompt)



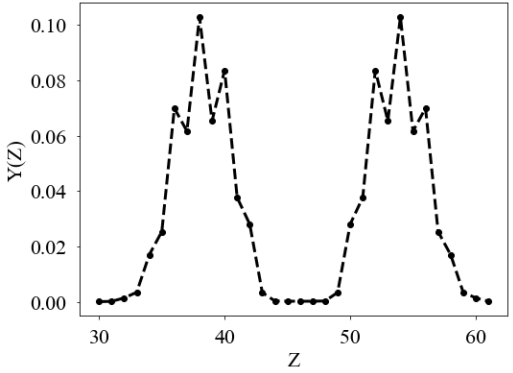
- Pre-fission neutron energy spectra
- Mass, charge, and kinetic energy of fission yields

Initial conditions of the fission fragments are modeled phenomenologically, fit to available experimental data

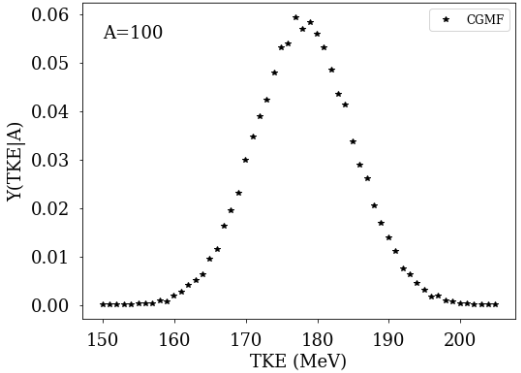
3 Gaussians



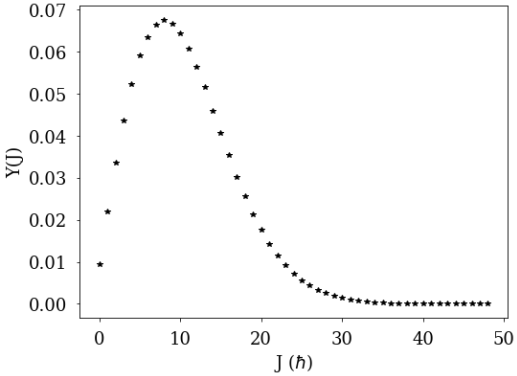
Wahl Systematics



Gaussian per mass



A.C. Wahl, LA-13928 (2002)



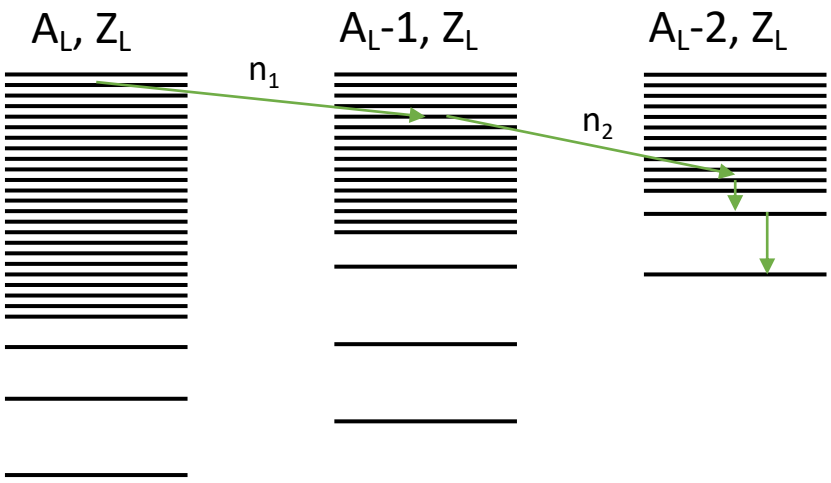
These initial conditions are essentially shared between the two codes – we can utilize optimization from one code for the other.

$$\rho(J) = \frac{1}{2}(2J+1)\exp\left[-\frac{J(J+1)}{2B^2}\right]$$

$$B^2 = \alpha\frac{\mathcal{I}_0(A,Z)T}{\hbar^2}$$

$$Y(A, Z, TKE, J, \pi)$$

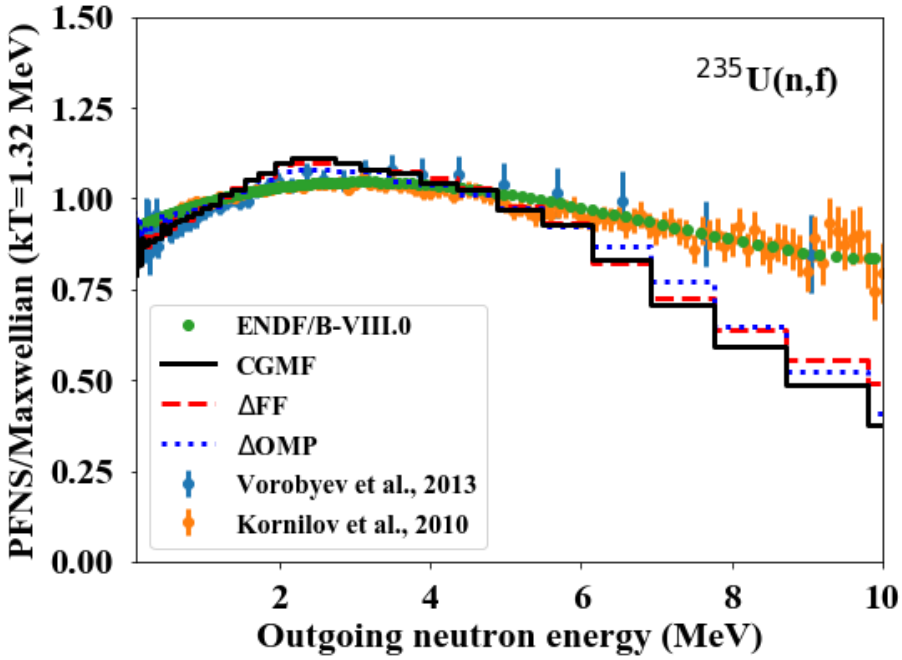
Additionally, many global models are needed in the de-excitation of the fission fragments



- Discrete nuclear levels (RIPL)
- Optical model potential (e.g. Koning Delaroche)
- Level densities
- Nuclear masses

Many models are constrained by experimental data, which is plentiful closer to the stable nuclei – not the case for the excited nuclei that are created during the fission process

Historically, the PFNS has been a challenge to reproduce with any Hauser-Feshbach decay model



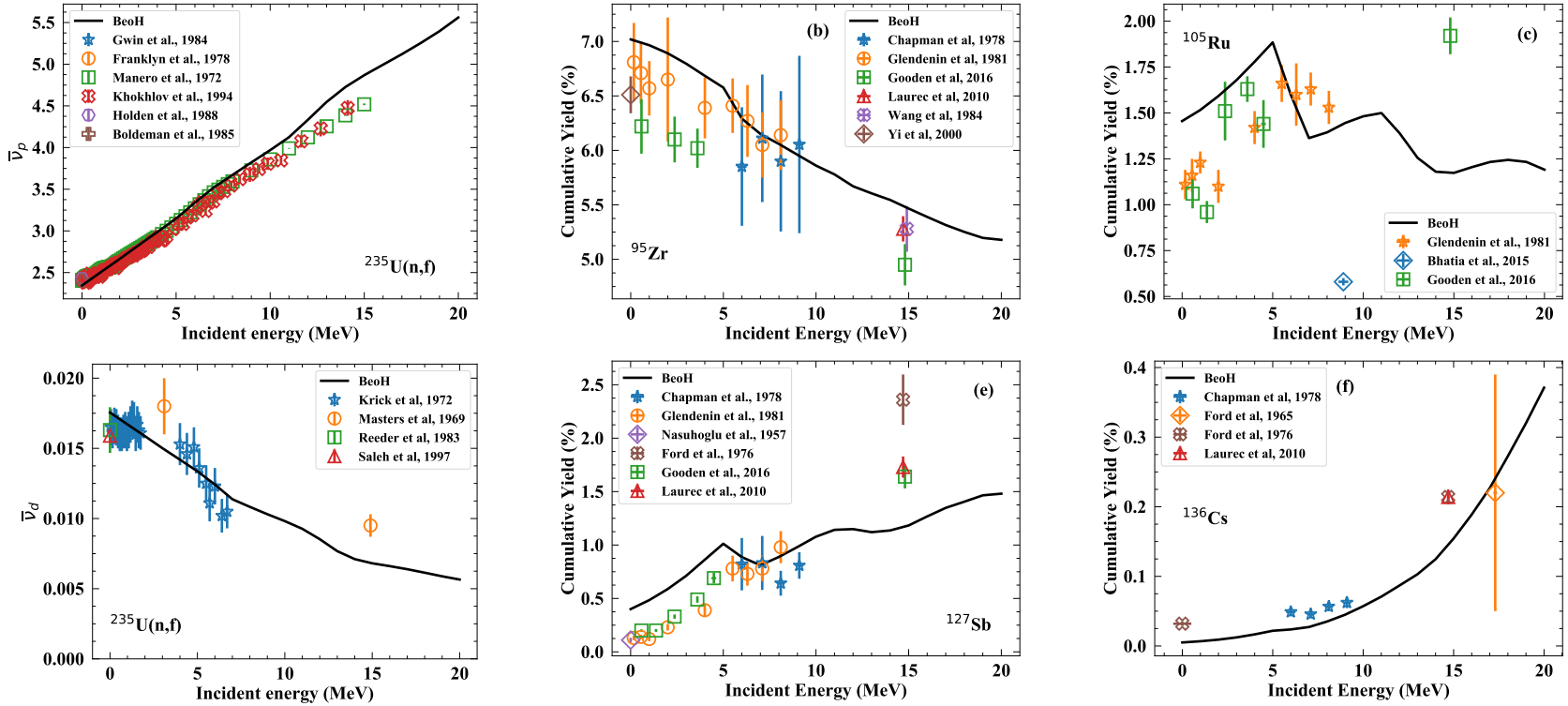
Changes to the fission fragment initial conditions that stay within the bounds of other observables (e.g. Y(A), TKE, multiplicities) can only move the PFNS so far.

In FY21 towards the current milestones, we spent a significant amount of time exploring different global models within CGMF and BeoH to improve the quality of the PFNS:

LA-UR-21-30882

Kawano, *et al.*, *PRC* **104**, 014611 (2021)

Average neutron multiplicities and fission product yields can be reproduced simultaneously (BeoH)



Lovell, Kawano, *et al.*, *PRC* **103** 014615 (2021)

Evaluation

- Evaluation technique
- Estimating experimental uncertainties in detail

We get evaluated data and covariances with GLLS using model data as a prior and updating with exp. info.

GLLS combines:

- **Model ("M") mean values and covariances,**
- **Experimental mean values ("x")** and covariances,
- **To evaluated mean values and covariances ("post") for a ND file** using,
- The design matrix S that either transforms from model parameter space to observable space or from energy lattice of the model to exp. one.

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

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

As prior, we either use information from CGMF or Los Alamos model.

Exp. database & covariances are obtained with the code *ARIADNE*

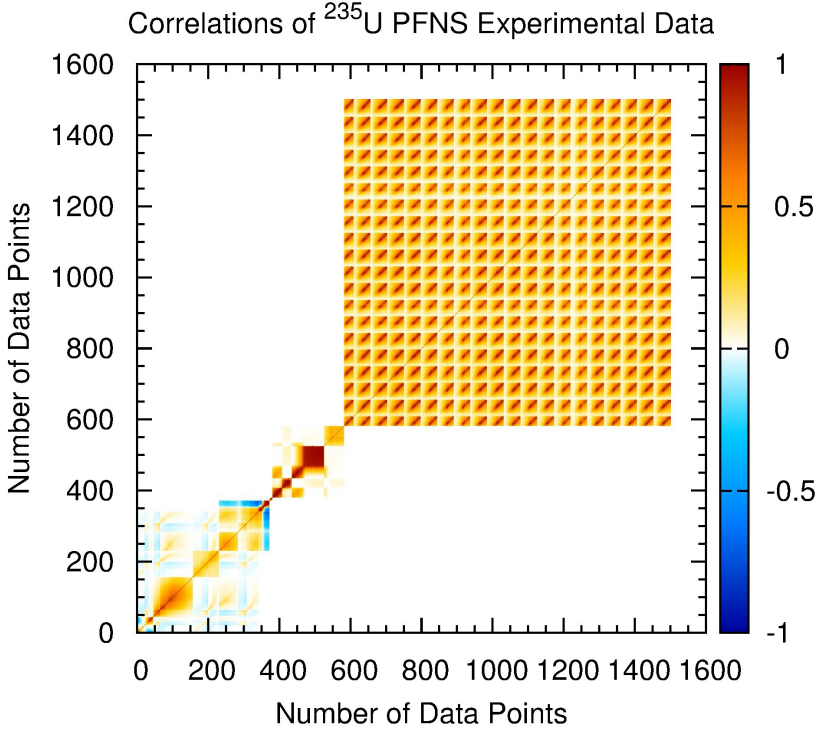
ARIADNE modules:

- PFNS exp. UQ,
- Nu-bar exp. UQ,
- (n,f) cross section UQ,
- Evaluations (Kalman, GLLS),
- Creating databases for evaluations in json, txt, previously xml.

UQ done:

- Implements templates of exp. unc. & unc./ metadata from EXFOR.
- A python notebook exists for each exp.

DN, EPJN 4, 34 (2018).

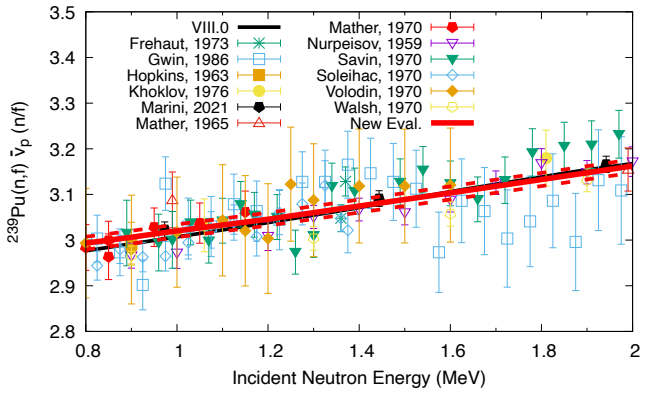


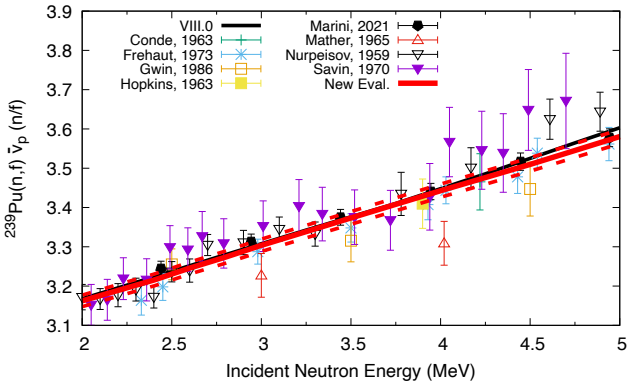
VIII.0 exp. cov. estimated with *ARIADNE*.

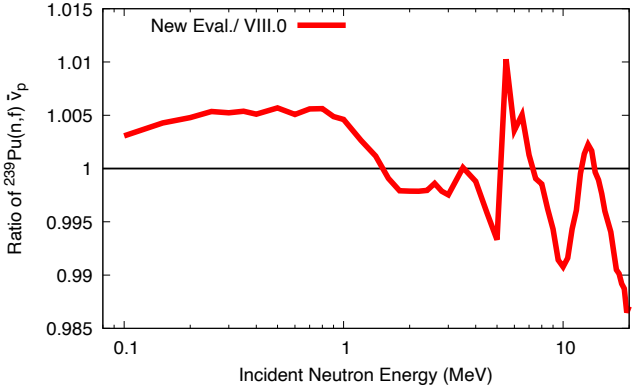
Evaluation

- Milestone: ^{235}U, ^{239}Pu: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (DUE FY22 Q4)

We have for the first time produced ENDF/B-quality nu-bar using CGMF. *Eval. ^{239}Pu nu-bar is in 2 VIII.1beta files!*







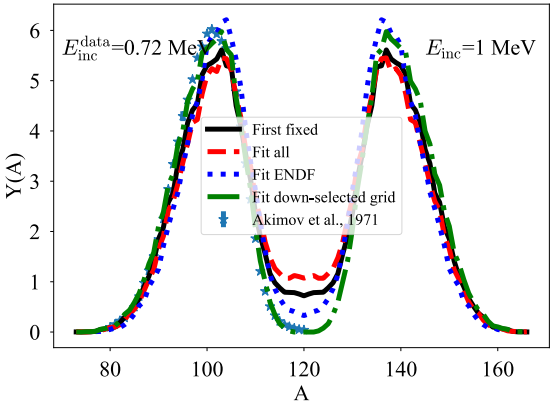
<u>Difference to ENDF/B-VIII.0:</u>

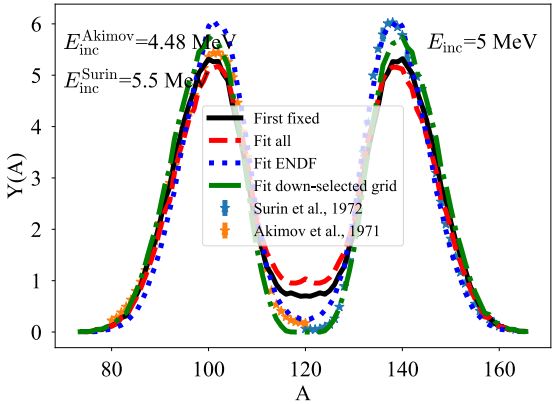
(a) New high-precision data by Marini (CEA) using Chi-Nu array,

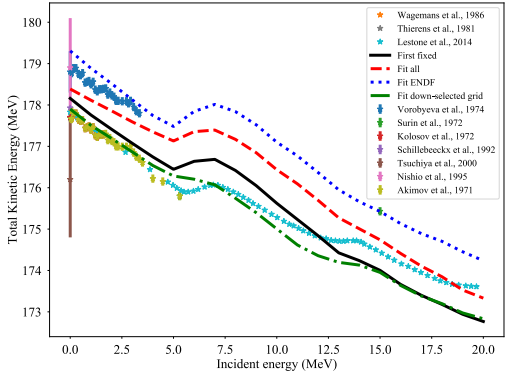
(b) improved UQ of past experimental data (template of expected exp. unc.),

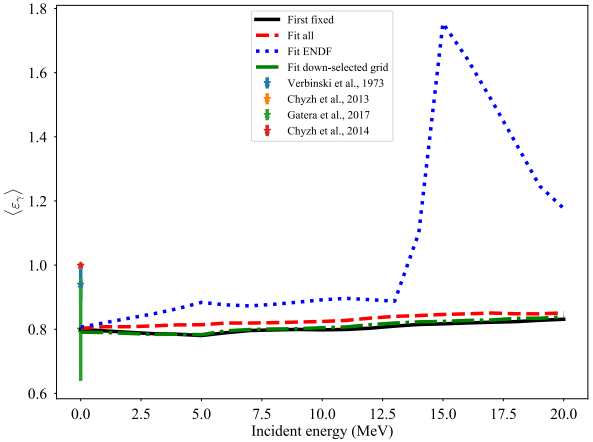
(c) using CGMF modeling consistent with TKE, FY, etc.

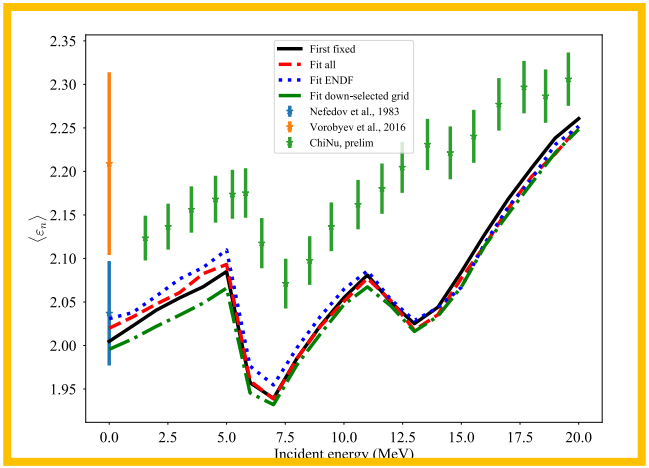
The eval. parameters of ^{239}Pu(n,f) nu-bar produce realistic estimates of fission quantities with CGMF.







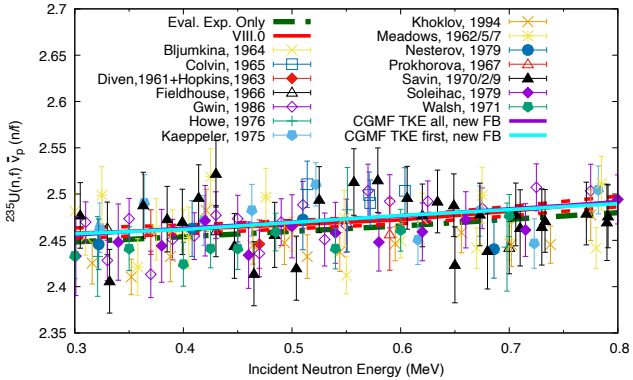


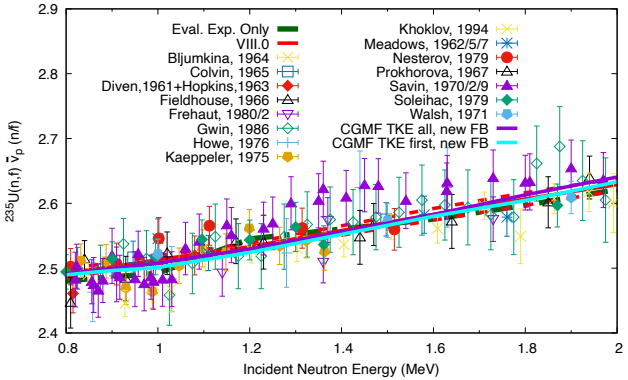


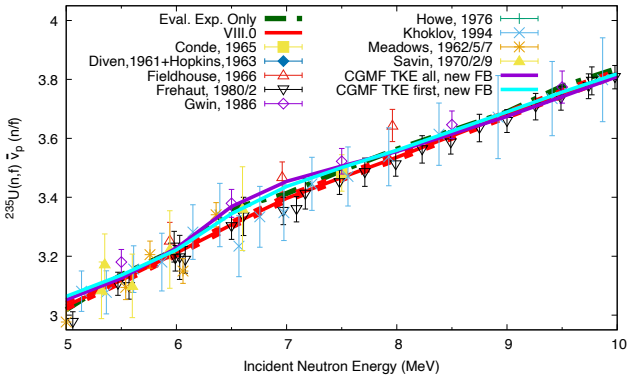
The only problem is that the PFNS is predicted too soft.

Produced ^{235}U nu-bar with CGMF that we test now for release.

Required detailed studies of <TKE> & fission barriers.







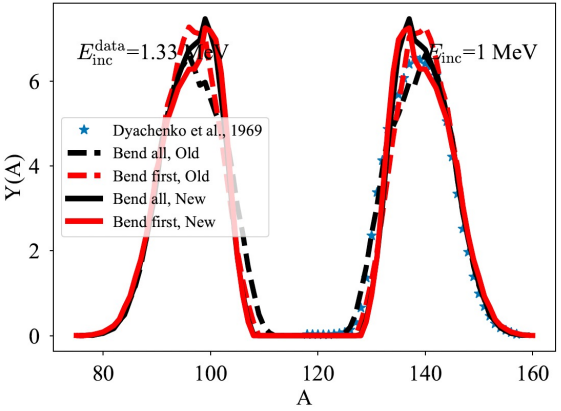
<u>Difference to ENDF/B-VIII.0:</u>

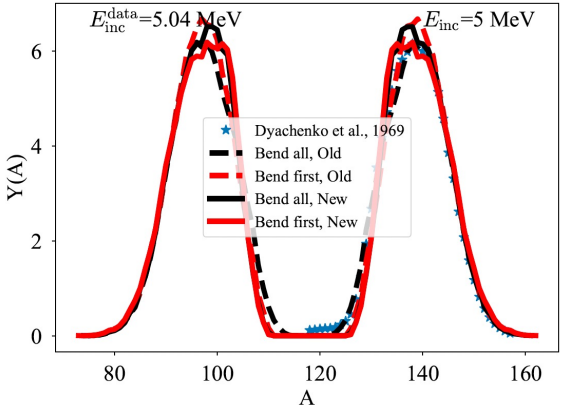
a) Included 2 new data sets (Boikov, Khoklov),

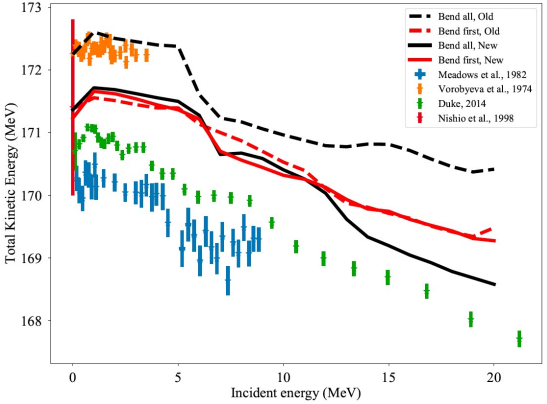
b) Improved UQ of past experimental data (template of expected exp. unc.),

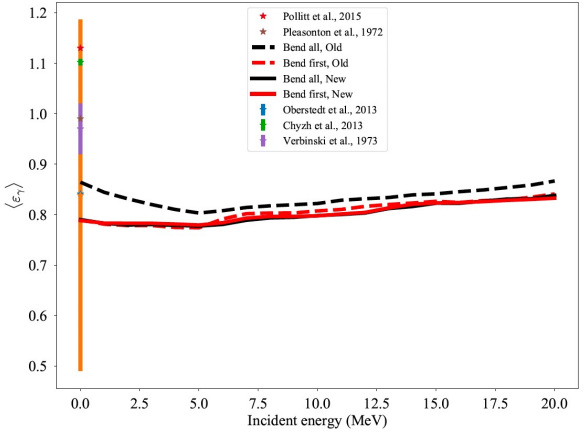
c) Using CGMF modeling consistent with TKE, Y(A), etc.

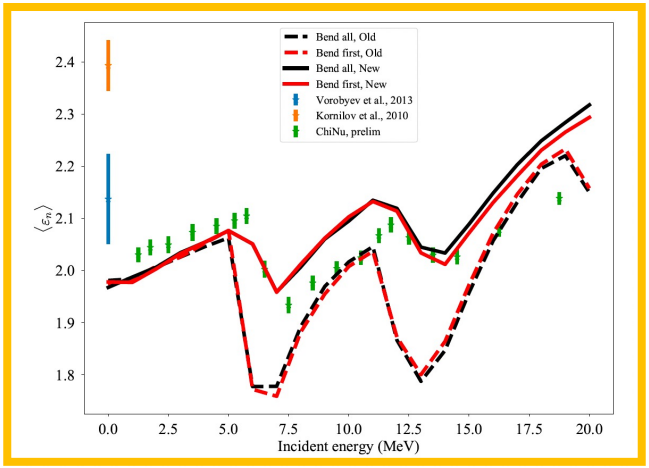
The eval. parameters of ^{235}U(n,f) nu-bar also produce realistic estimates of fission quantities with CGMF.





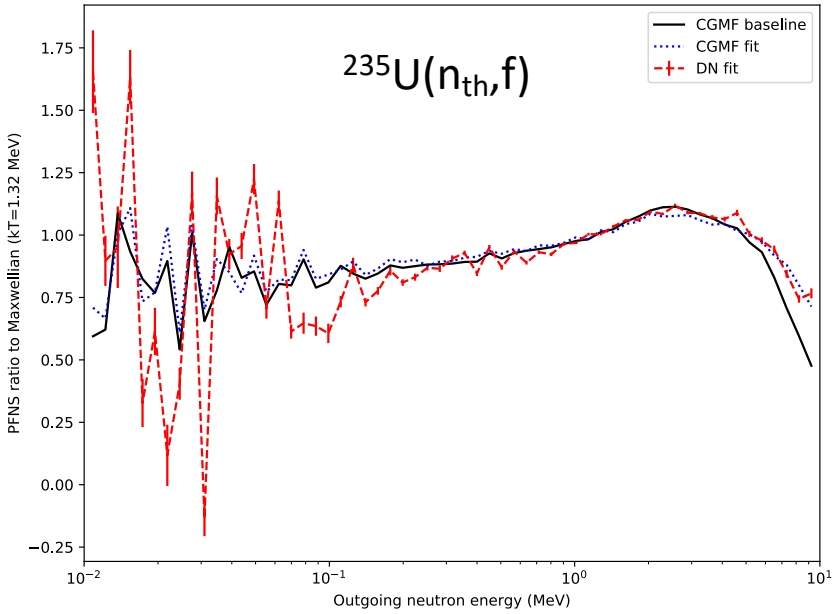


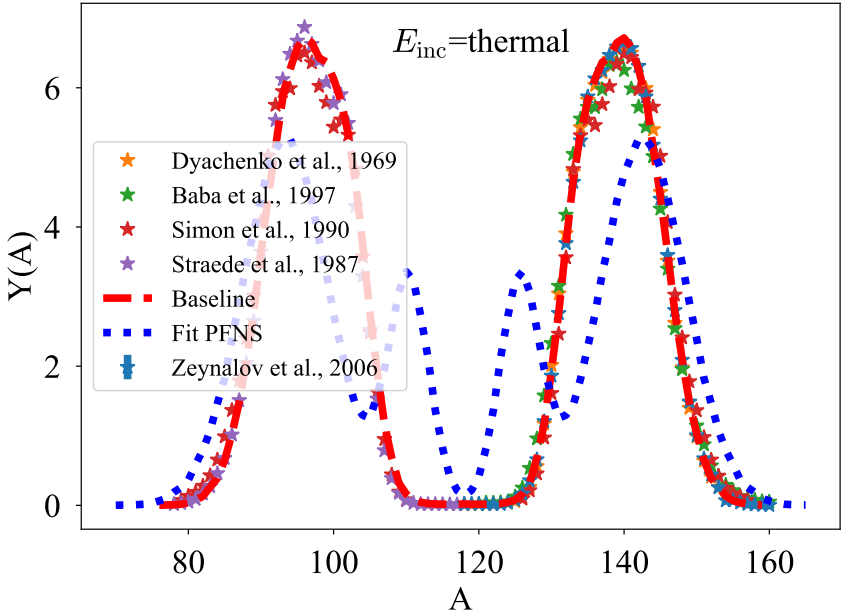




The PFNS seems to agree better than for ^{239}Pu BUT …

Kalman optimization of the PFNS with baseline CGMF either produces unphysical PFNS or parameters.





We can produce PFNS together with nu-bar using CGMF.

If we want ENDF/B-quality evaluated PFNS we still need to use the Los Alamos model.

Evaluation

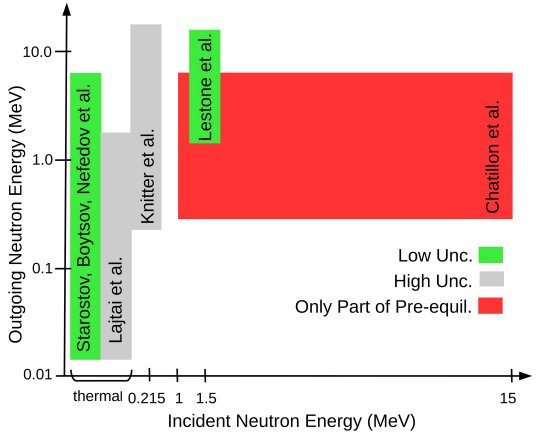
- Milestone: ^{235}U: “Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu” -> we did that also for ^{239}Pu

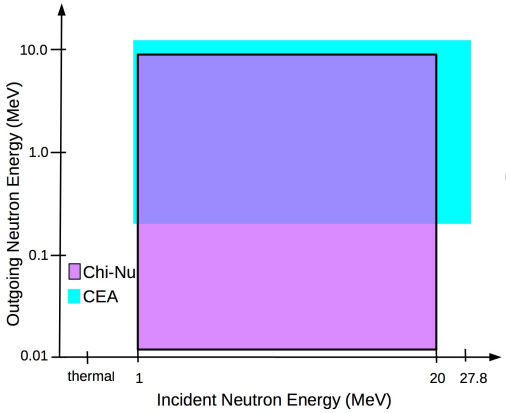
High-precision ^{239}Pu & ^{235}U PFNS by Chi-Nu significantly expanded our database!

VIII.0 Database

Additional data (FY21/22)

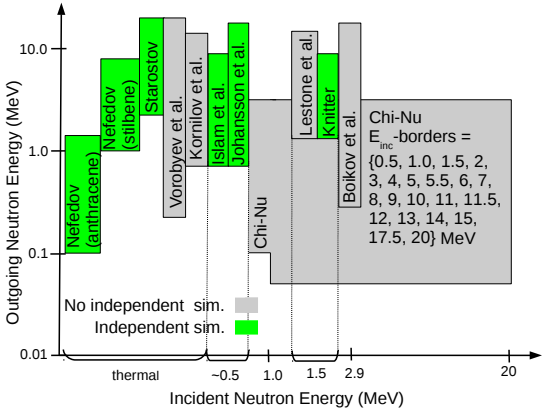
^{239}Pu

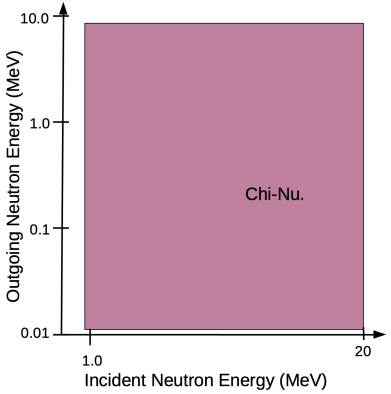




→ Both data sets were taken at LANSCE with the Chi-Nu array as part of a NNSA/CEA collaboration.

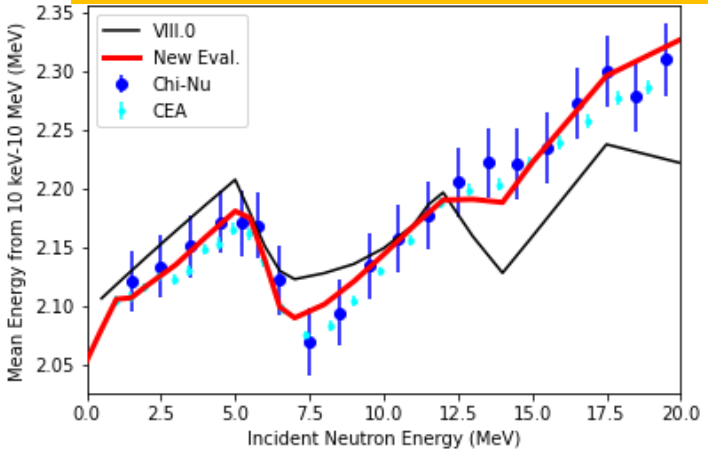
^{235}U

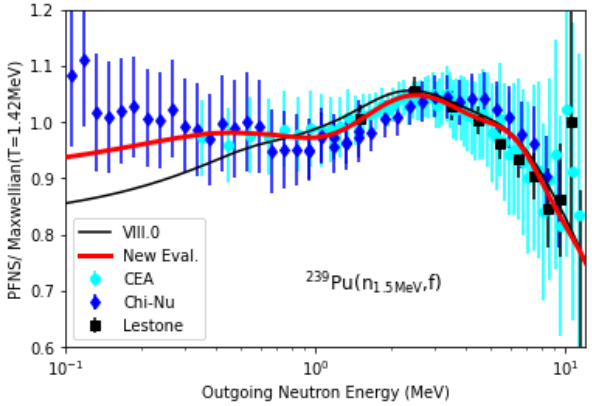


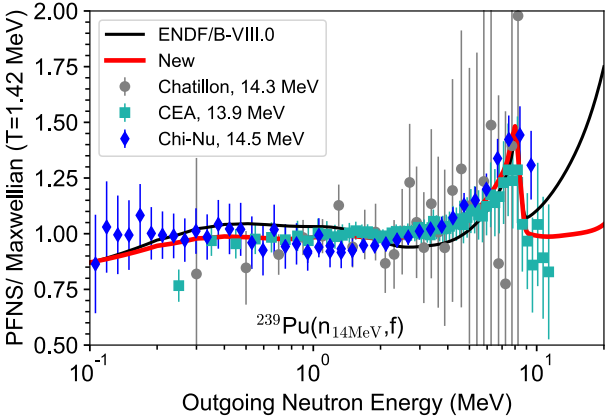


→ New Chi-Nu data is completely re-analyzed, has higher precision and goes up to E_{out} =10 MeV instead of 2 MeV.

Eval. ^{239}Pu PFNS using Chi-Nu & CEA data and Los Alamos model are in 2 VIII.1beta files!



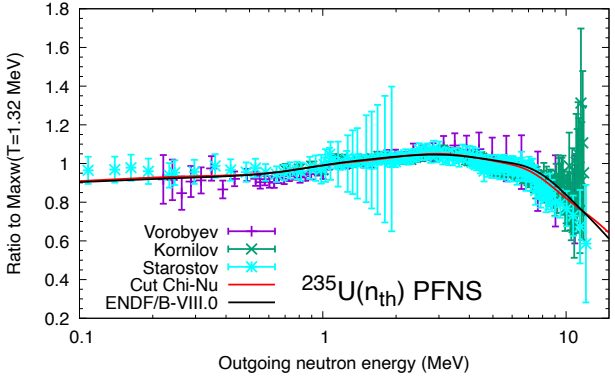


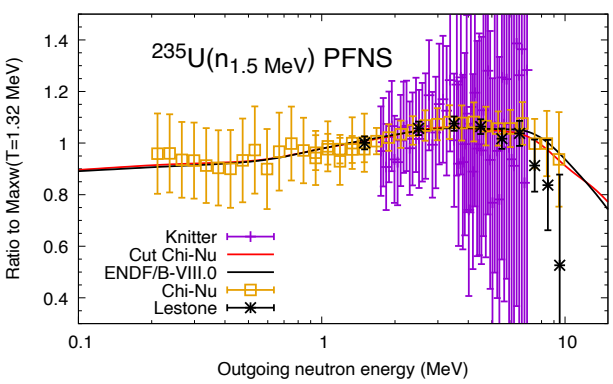


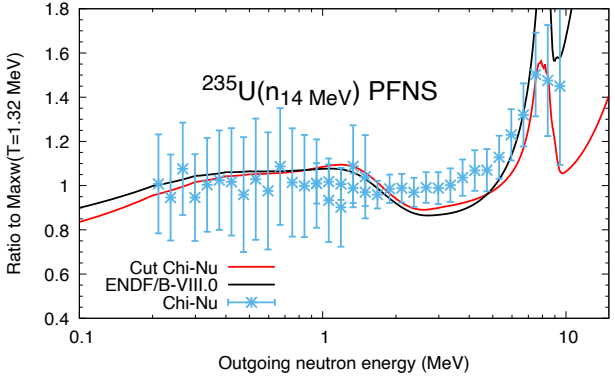
(a) <u>Difference to VIII.0:</u>New high-precision PFNS by Chi-Nu & CEA,
(b) <u>Same as VIII.0:</u>Used the Los Alamos model (DN et al., NDS 148, 293 (2018)).

We test eval. ^{235}U PFNS using Chi-Nu data now for release.

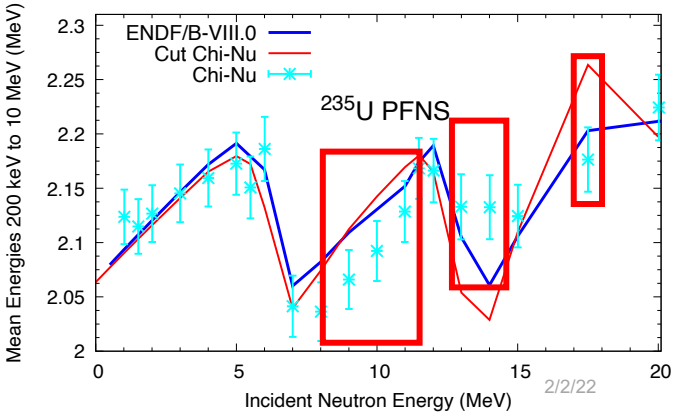
Some work needs to be done for E_{inc} > 7 MeV







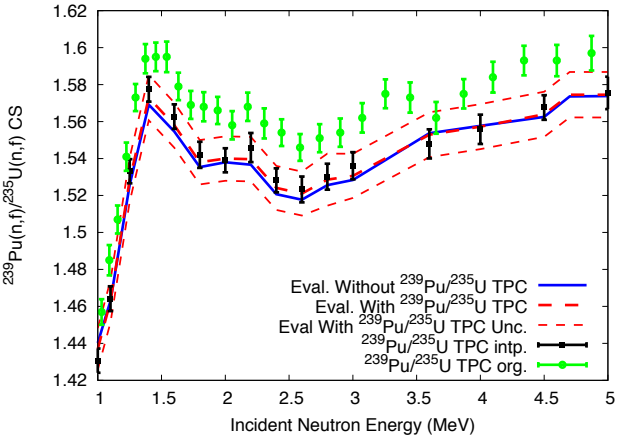
- The new eval. corresponds well to independent INDEN eval. at thermal.,
- Eval. agrees well with Chi-Nu E_{inc} = 1-7 MeV,
- Some work needed at E_{inc}={8-11,13-14} MeV.

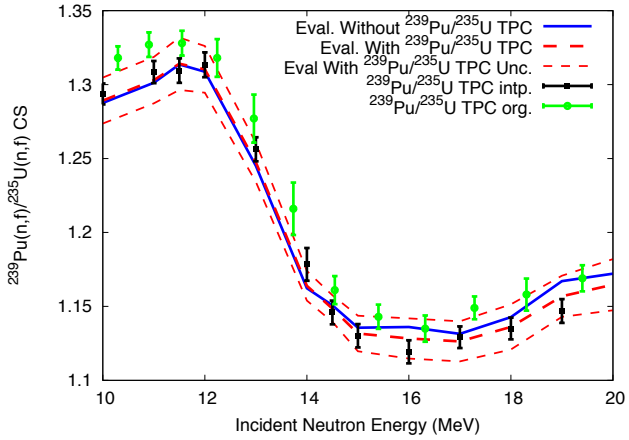


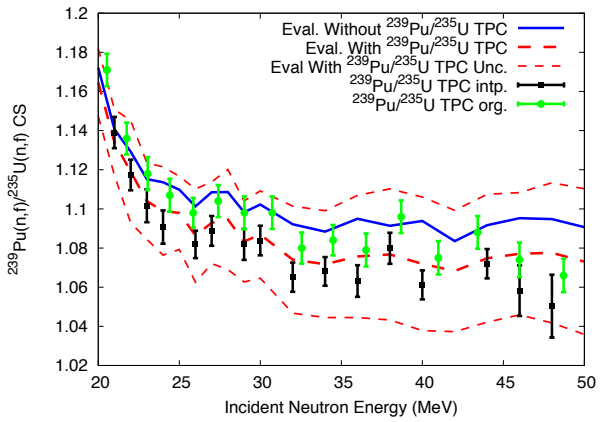
Evaluation

- Milestone: ^{239}Pu, ^{235}U: “Update fission cross section based on TPC results (from ^{239}Pu/^{235}U ratio data)” (DUE FY21 Q4).

^{239}Pu/^{235}U(n,f) niffteTPC data were included in standards eval. The eval. data are now in 2 VIII.1beta files!





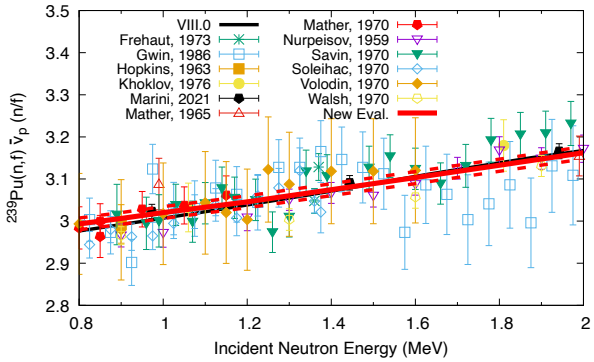


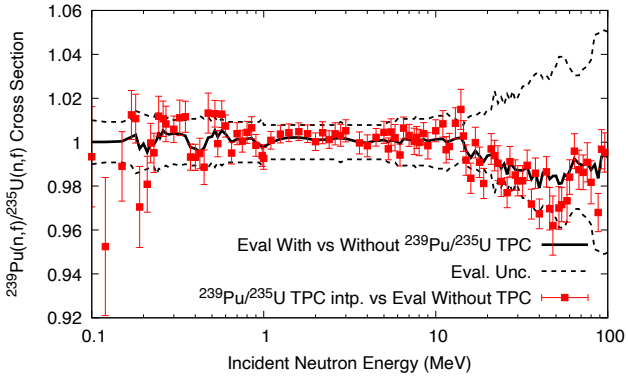
fissionTPC data change the evaluation significantly above 10 MeV and raised some questions on past data that the standards committee are now exploring.

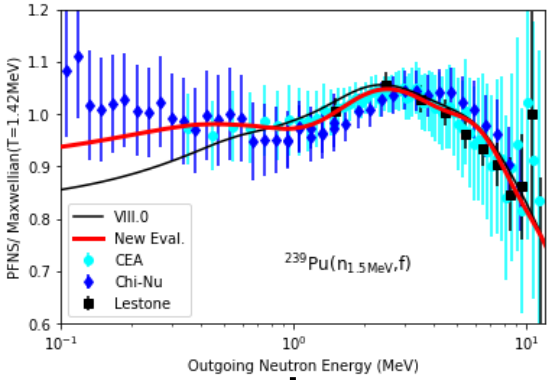
- TPC intp … TPC data after standard interpolation, and normalization procedure.
- TPC org … as reported by niffteTPC collaboration.
- Eval. Without TPC … current standard file.

Many changes in ^{239}Pu, but they work well together!

Change from ENDF/B-VIII.0 to VIII.1 beta1







Change in Jezebel k_{eff}*

+ 139 pcm

-40 pcm

-121 pcm

Total change: - 22 pcm (from 1.00069 -> 1.00047) -> all good.

The combination of the new nu-bar, PFNS and fission cross section give a realistic k_{eff} of Jezebel! More changes coming for other cross sections.

*Change of 220 pcm in Jezebel k_{eff} – range between prompt & delayed critical, k_{eff} unc: 123 pcm.

Summary

- Currently in VIII.1 LANL and IAEA test files:
  - ^{239}Pu nu-bar including CGMF modeling and CEA data,
  - ^{239}Pu PFNS including Chi-Nu & CEA data,
  - ^{239}Pu(n,f) cross section including fissionTPC data.
- Currently being tested if fit for release:
  - ^{235}U nu-bar including CGMF modeling,
  - ^{235}U PFNS including Chi-Nu data.

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To-Do:

- Correct ^{235}U Chi-Nu PFNS at higher E_{inc},
- Benchmark ^{235}U PFNS & nu-bar evaluations,
- Get ^{238}U nu-bar.

Thank you for your attention!

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