Los Alamos
NATIONAL LABORATORY

Evaluations for ^{235,238}U and ^{239}Pu fission-source term observables

Amy Lovell & Denise Neudecker

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LA-UR-23-21415

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

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

FY22-23 milestones:

- ^{235}U, ^{239}Pu: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4),
- ^{235}U: “Develop consistent evaluation of fission yields, neutron multiplicity, and spectra from thermal to 20 MeV” (FY22 Q4)
- ^{238}U: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4),
- ^{235}U: “Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu” (FY22 Q2),
- ^{238}U: “Finalize prompt fission neutron spectra based on LANSCE Chi-Nu Data” (FY23 Q4),
- $^{238,240\text{-}242}$Pu: “Attempt a consistent nu-bar evaluation supported by a model code to provide better evaluated nu-bar for minor Pu-isotopes” (FY23 Q4).

FY22-23 milestones:

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- $^{238,240\text{-}242}$Pu: “Attempt a consistent nu-bar evaluation supported by a model code to provide better evaluated nu-bar for minor Pu-isotopes” (FY23 Q4).

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

Modeling and related milestones

- Milestone: ^{235}U: “Develop consistent evaluation of fission yields, neutron multiplicity, and spectra from thermal to 20 MeV” (FY22 Q4)
  - Lovell, Kawano, *et al*., *PRC* **103** 014615 (2021)
- Milestone: $^{238,240\text{-}242}$Pu: “Attempt a consistent nu-bar evaluation supported by a model code to provide better evaluated nu-bar for minor Pu-isotopes” (FY23 Q4).
  - Lovell and Neudecker, LA-UR-22-29570

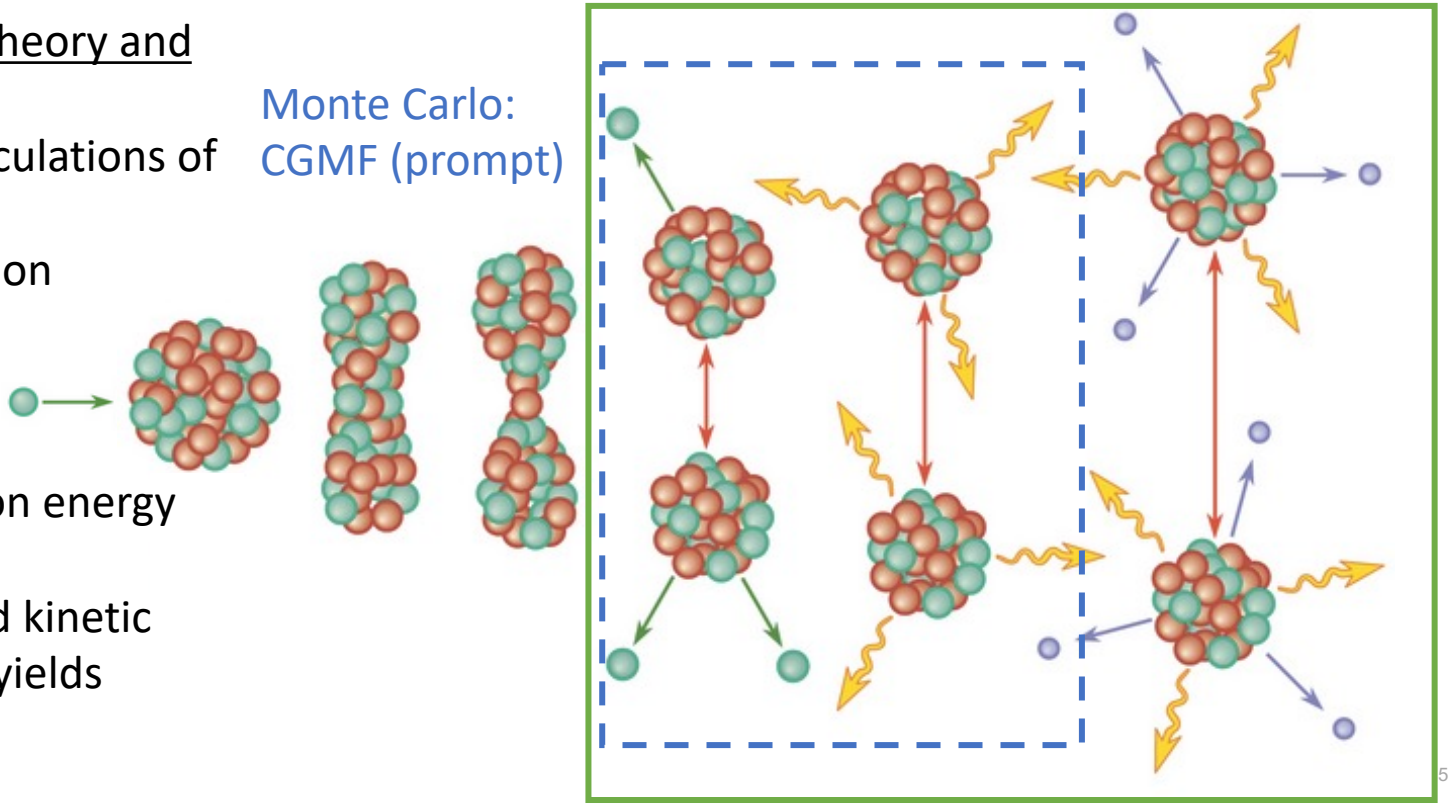
Monte Carlo and deterministic models at LANL

Deterministic: BeoH (prompt and delayed)

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

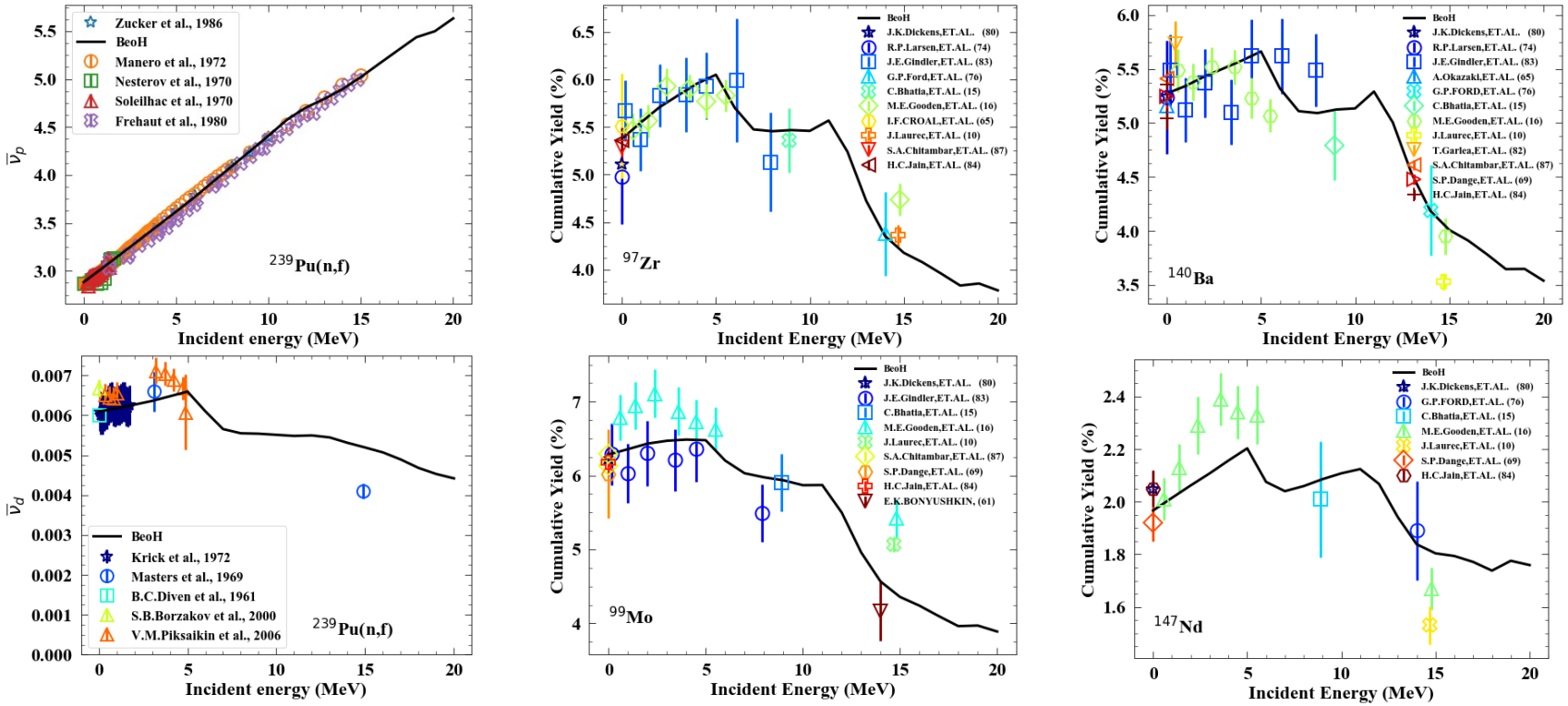
- First-principle calculations of fission yields
- Multi-chance fission probabilities

Monte Carlo:
CGMF (prompt)



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

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

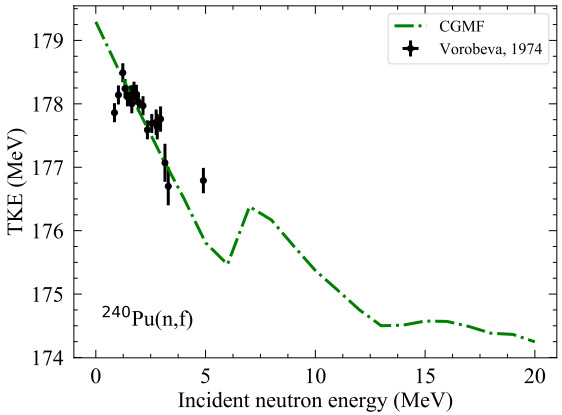


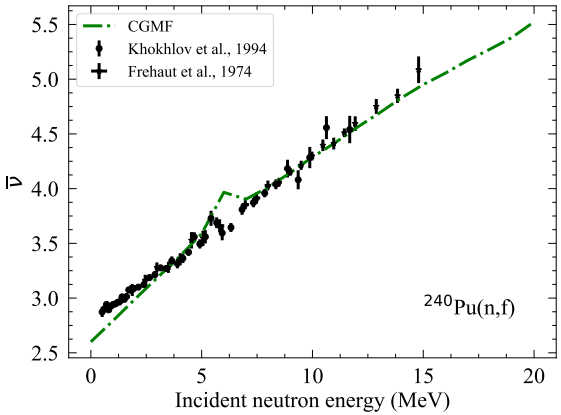
Lovell, Kawano, *et al.*, *PRC* **103** 014615 (2021)

Consistency among Pu isotopes is being developed (CGMF, towards FY23 milestone)

^{239}Pu(n,f) and ^{241}Pu(n,f) are already included in CGMF. The parametrizations can be interpolated to calculate ^{240}Pu(n,f). First results – without any optimization – are promising.

Lovell and Neudecker, LA-UR-22-29570





TKE and neutron multiplicity already agree reasonably well with experimental data

Evaluation and related milestones

- Milestone: ^{235}U, ^{239}Pu: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4):
  - ^{239}Pu nu-bar, PFNS and (n,f) cross section: Neudecker, Lovell et al., Frontiers in Physics Vol. 10, (2022); https://doi.org/10.3389/fphy.2022.1056324
  - ^{235}U nu-bar: Lovell, Neudecker, Talou, LA-UR-22-23475
  - ^{235}U PFNS: Lovell and Neudecker, LA-UR-22-29989 (2022).

- Milestone: ^{238}U: “Evaluate PFNS and multiplicity consistently, including angular information about prompt neutrons” (FY22 Q4):
  - Neudecker, Lovell, Kawano and Talou, LA-UR-22-29906

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

GLLS combines:

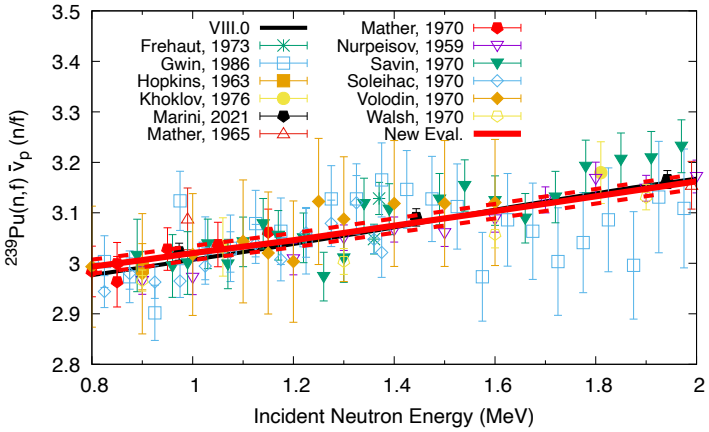
- **Model ("M") mean values and covariances,**
- **Experimental mean values ("x")** and covariances,
- **To evaluated mean values and covariances ("post") for a ND file** using,
- The design matrix S that either transforms from model parameter space to observable space or from energy lattice of the model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

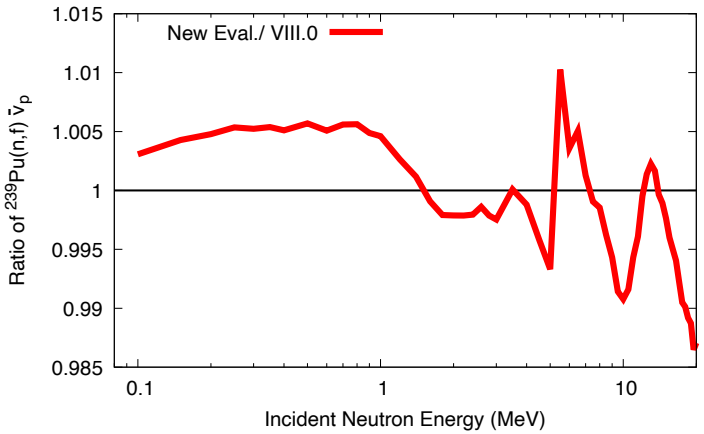
$$\underline{\phi}^{post} = \underline{\phi}^{M} + \mathbf{Cov}^{post}\mathbf{S}^{+}\left(\mathbf{Cov}^{x}\right)^{-1}\left(\underline{\phi}^{x} - \mathbf{S}\underline{\phi}^{M}\right),$$

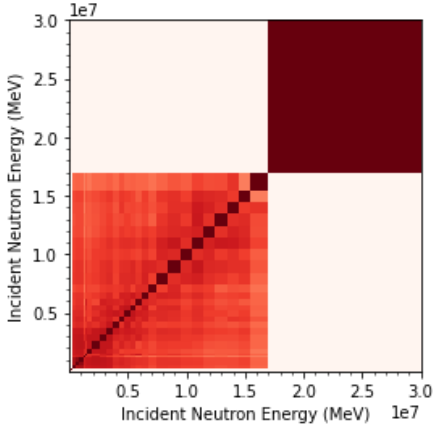
$$\mathbf{Cov}^{post} = \mathbf{Cov}^{M} - \mathbf{Cov}^{M}\mathbf{S}^{+}\left(\mathbf{S}\mathbf{Cov}^{M}\mathbf{S}^{+} + \mathbf{Cov}^{x}\right)^{-1}\mathbf{S}\mathbf{Cov}^{M}$$

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

We produced for the first time ENDF/B-quality nu-bar using CGMF. *Eval. ^{239}Pu nu-bar and cov in VIII.1β1.*







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

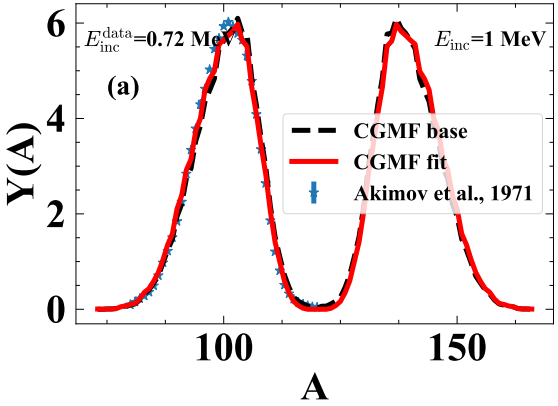
(a) New high-precision data by Marini (CEA) using Chi-Nu array,

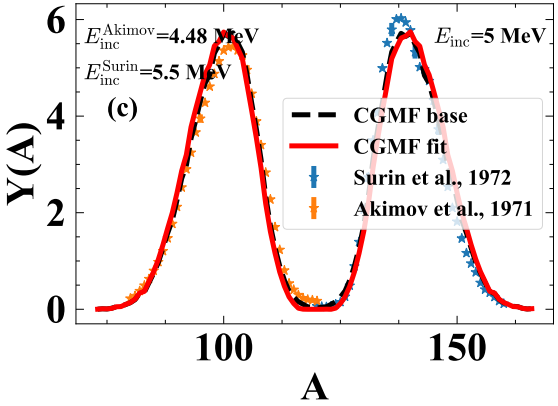
(b) improved UQ of past experimental data (template of expected exp. unc.),

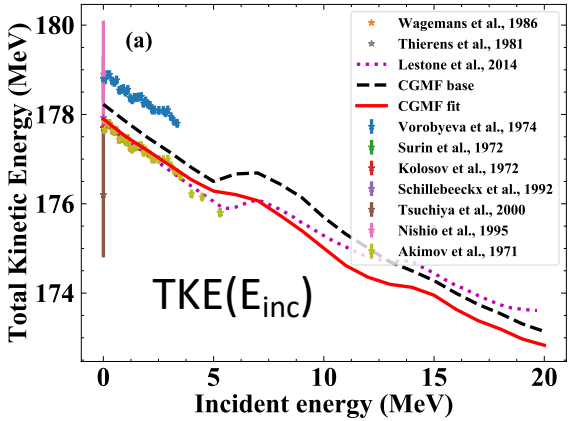
(c) using CGMF modeling consistent with TKE, FY, etc.

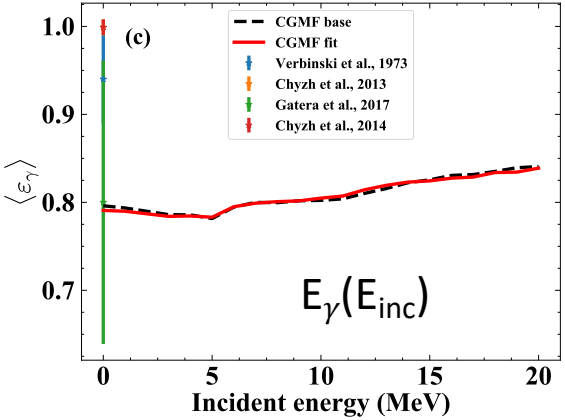
New compared to TPR 2022: covariances supplied.

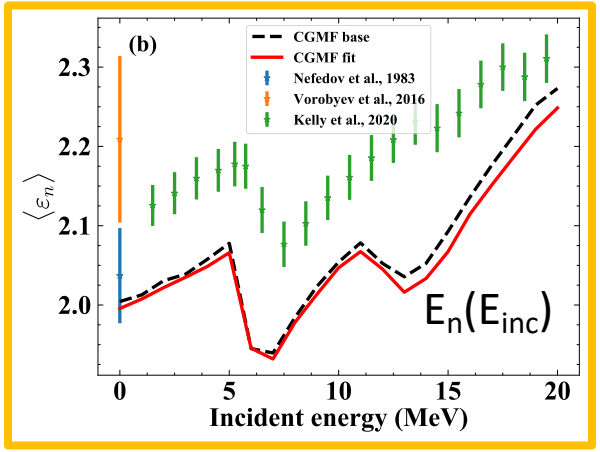
The eval. parameters of ^{239}Pu(n,f) nu-bar produce realistic estimates of fission quantities with CGMF.





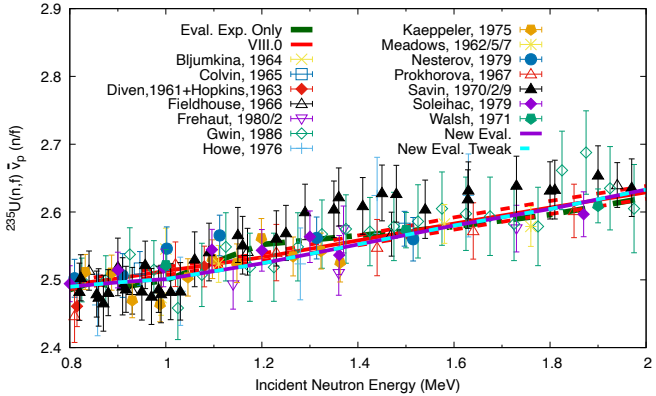


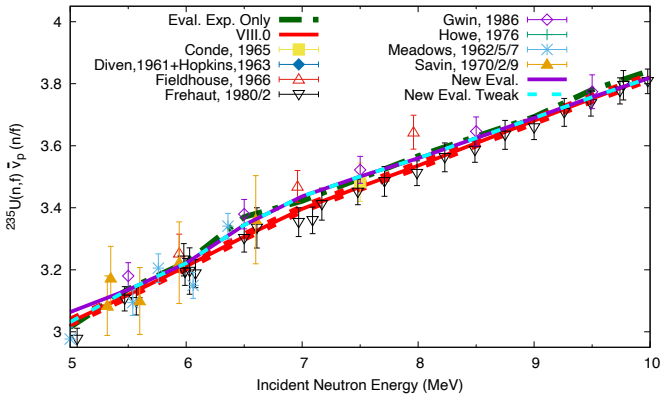


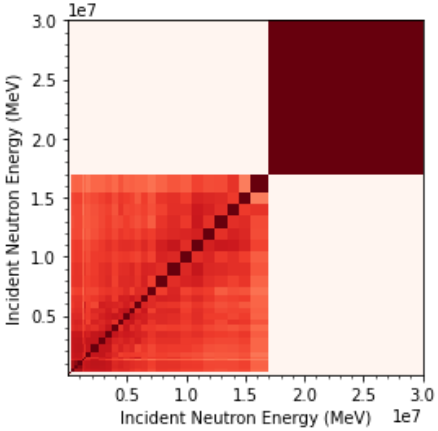


The only problem is that the PFNS is predicted too soft.

We produced also ENDF/B-quality ^{235}U nu-bar using CGMF. *Eval. ^{235}U nu-bar and cov in VIII.1β1.*







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

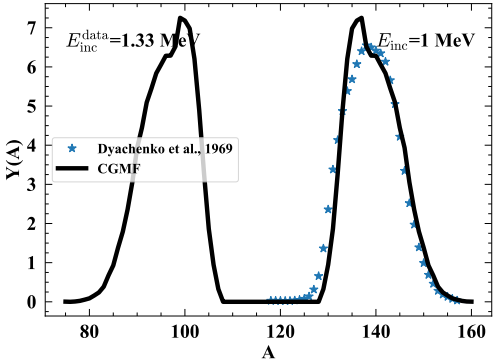
a) Included 2 new data sets (Boikov, Khoklov),

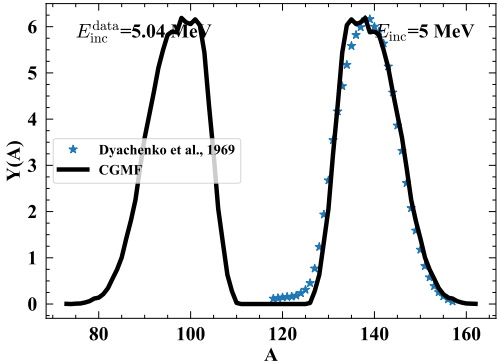
b) Improved UQ of past experimental data (template of expected exp. unc.),

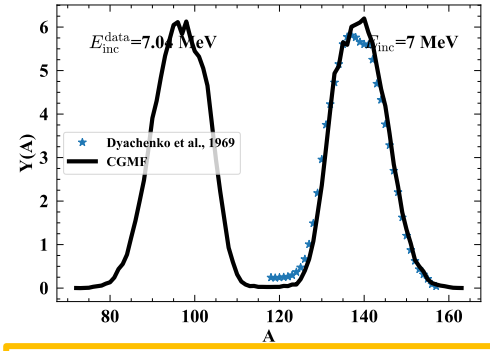
c) Using CGMF modeling consistent with TKE, Y(A), etc.

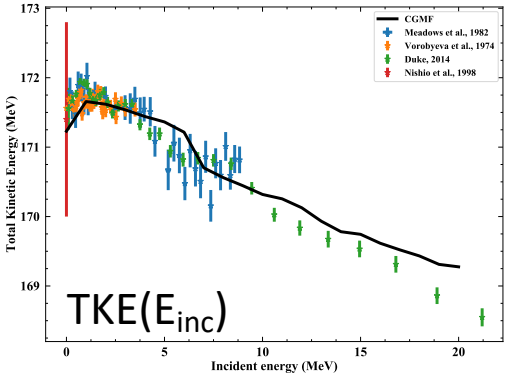
New compared to TPR 2022: data finalized & accepted, covariances supplied.

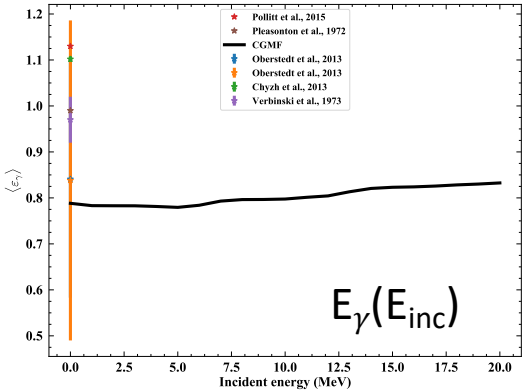
The evaluated parameters link favorably back to other fission quantities, except for PFNS, using CGMF.

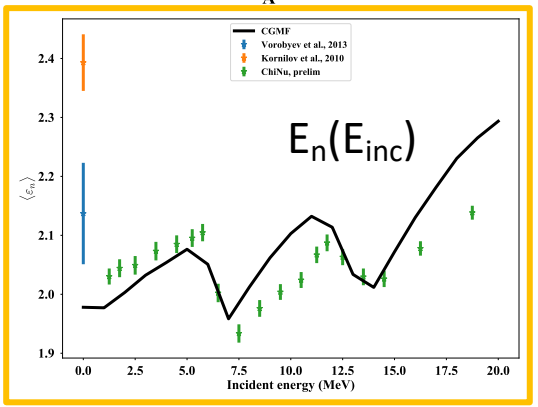






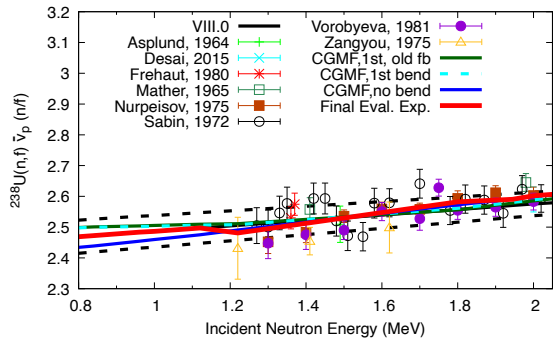


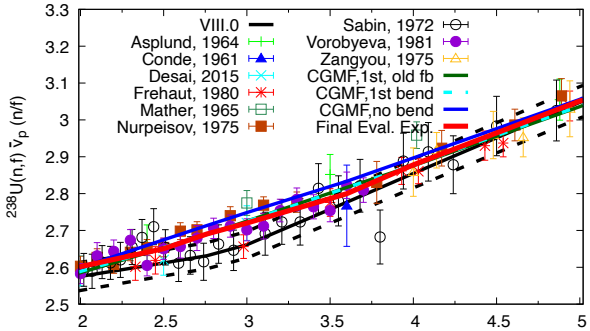


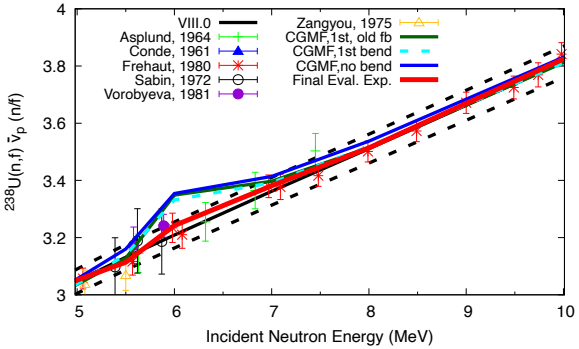


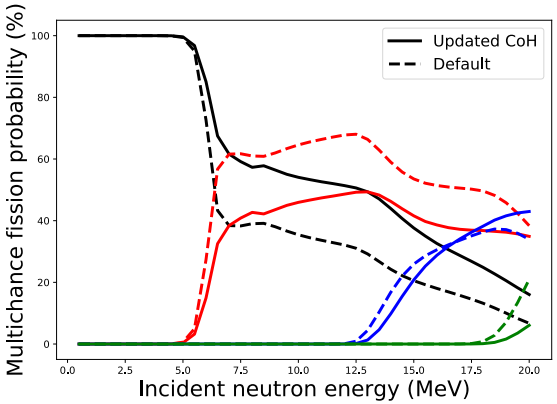
Using CGMF for evaluations brings the added benefit that we can link back nu-bar to Y(A), TKE(A), etc. to see if they are all consistent and realistic.

Evaluated ^{238}U nu-bar, with and without CGMF, differs from ENDF/B-VIII.0 from 2-4 MeV. New experimental data needed.









Need to counter-balance change in nu-bar by PFNS. Chi-Nu delivered FY23 data. nu-bar to be measured by CEA.

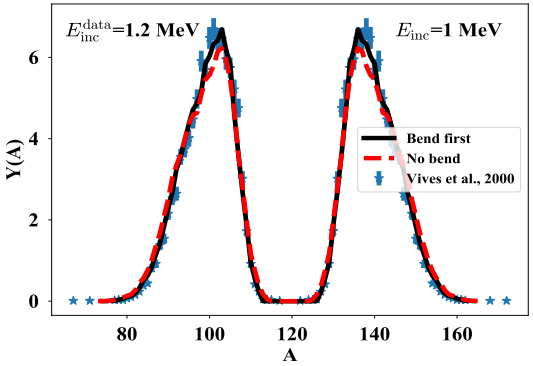
ENDF/B-VIII.0:

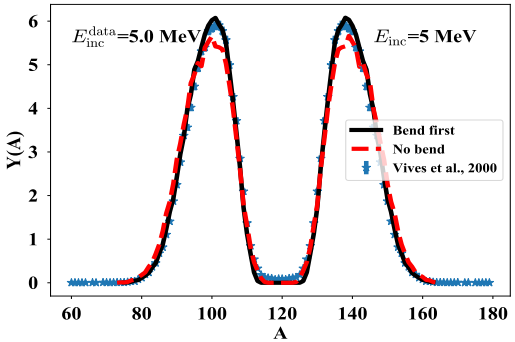
a) VIII.0 based on Frehaut, no detailed UQ of past data,

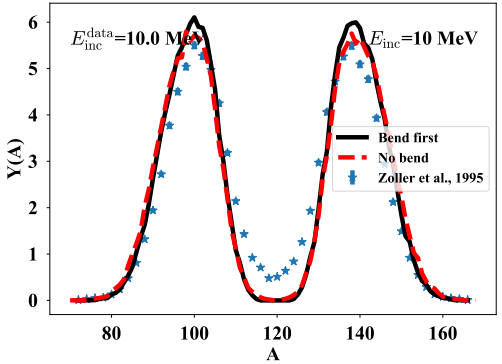
b) No model!

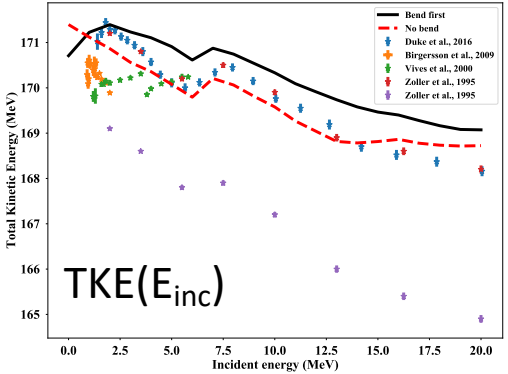
New compared to TPR 2022: completely new evaluation, modeling, exp UQ.

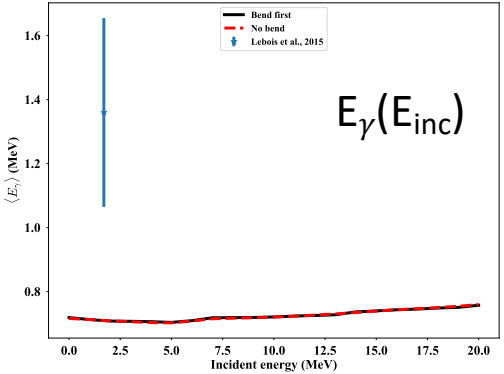
The evaluated parameters link favorably back to other fission quantities, except for PFNS, using CGMF.

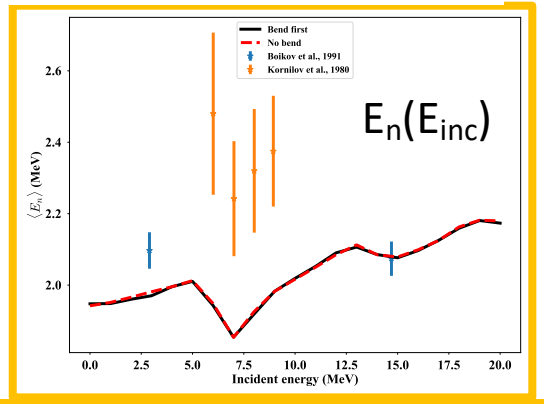












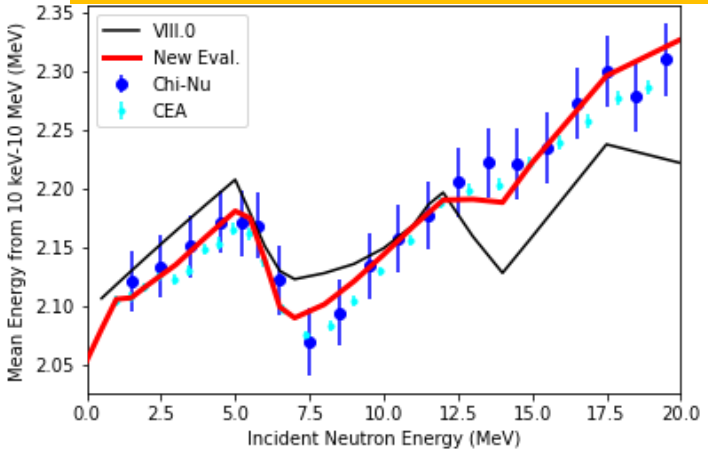
We are doing reasonably fine in describing Y(A), but <TKE> not as well-described (large spread in data). New experimental nu-bar will help.

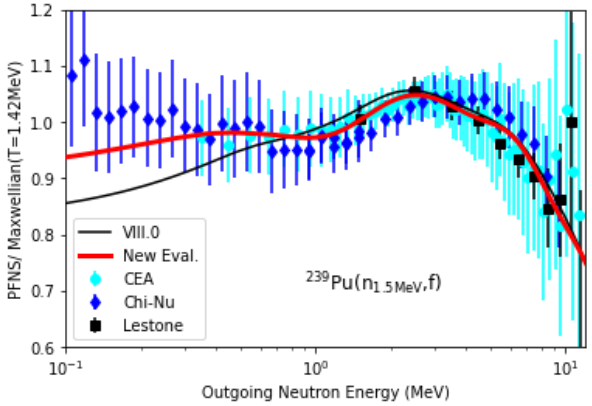
Evaluation

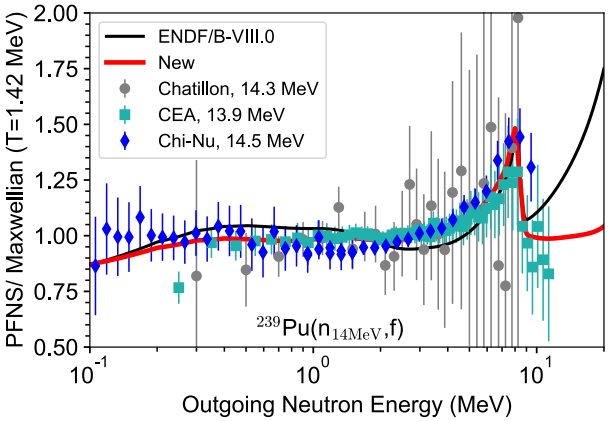
- Milestone: ^{235}U: “Finalize prompt fission neutron spectra based on LANSCE high-energy emission data from Chi-Nu” -> we did that also for ^{239}Pu
  - ^{239}Pu nu-bar, PFNS and (n,f) cross section: Neudecker, Lovell, Kelly, Marini, et al., Frontiers in Physics Vol. 10, (2022); https://doi.org/10.3389/fphy.2022.1056324
  - ^{235}U PFNS: Neudecker and Kelly, LA-UR-22-22220 (2022).

- Milestone: ^{238}U: “Finalize prompt fission neutron spectra based on LANSCE Chi-Nu Data” (FY23 Q4)
  - Keegan Kelly delivered data for evaluation to Denise Neudecker December 2022,
  - modeling, exp. UQ, and evaluation ongoing.

Eval. ^{239}Pu PFNS and cov using Chi-Nu & CEA data and Los Alamos model are in VIII.1β1.



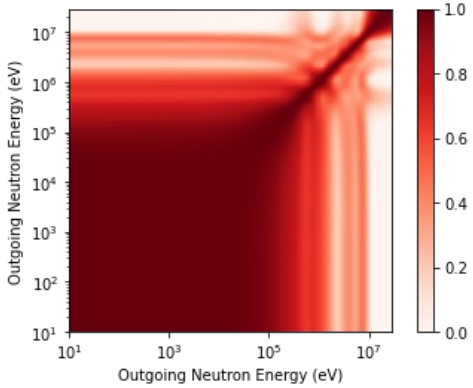




(a) <u>Difference to VIII.0:</u> High-precision Chi-Nu & CEA PFNS,

(b) <u>Same as VIII.0:</u>Los Alamos model (DN et al., NDS 148, 293 (2018)).

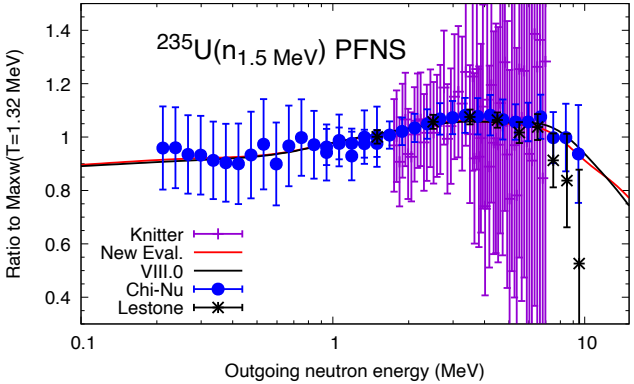
Mean energy uncertainty at E_{inc} = 1.5 MeV: 33.7 keV.

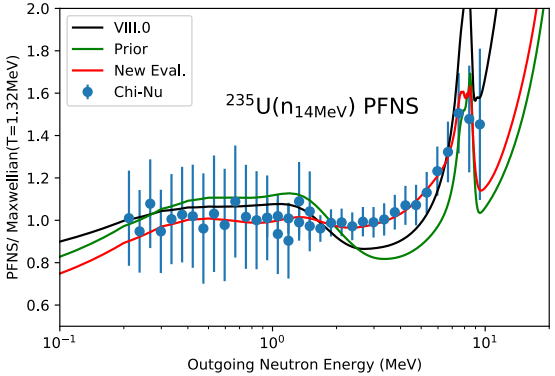


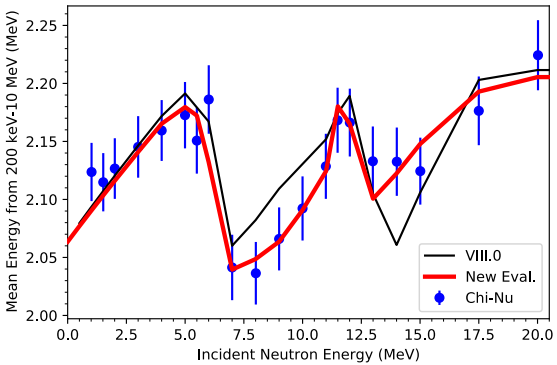
E_{inc} = 1.5 MeV

New compared to TPR 2022: covariances supplied.

Eval. ^{235}U PFNS and covariance using Chi-Nu data and Los Alamos model are in VIII.1β1.





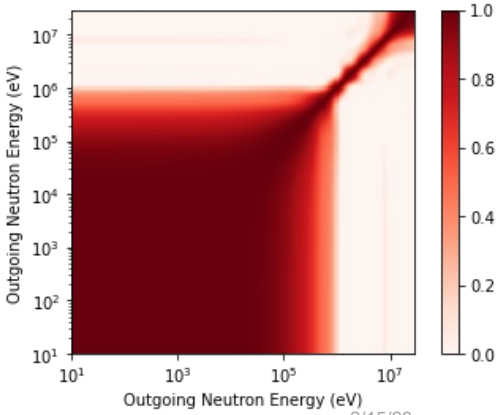


(a) <u>Difference to VIII.0:</u> All high-precision Chi-Nu PFNS,

(b) <u>Same as VIII.0:</u>Los Alamos model (DN et al., NDS 148, 293 (2018)).

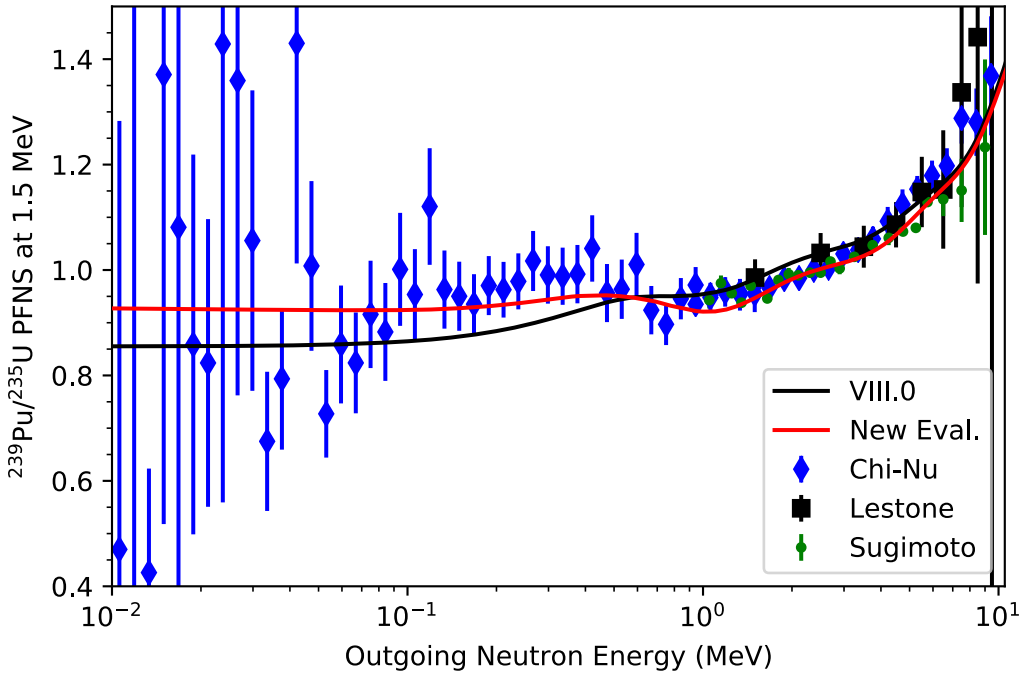
Mean energy uncertainty at E_{inc} = 1.5 MeV: 28 keV.

New compared to TPR 2022: PFNS finalized, data accepted, covariances supplied, benchmarking done.



E_{inc} = 1.5 MeV

Ratio of VIII.1$\beta 1$ ^{239}Pu/^{235}U(n,f) PFNS at E_{inc} = 1.5 MeV remains in good agreement with experimental data.

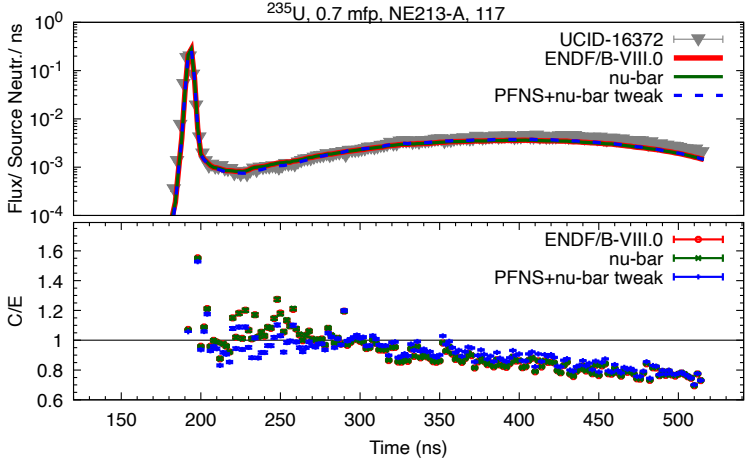


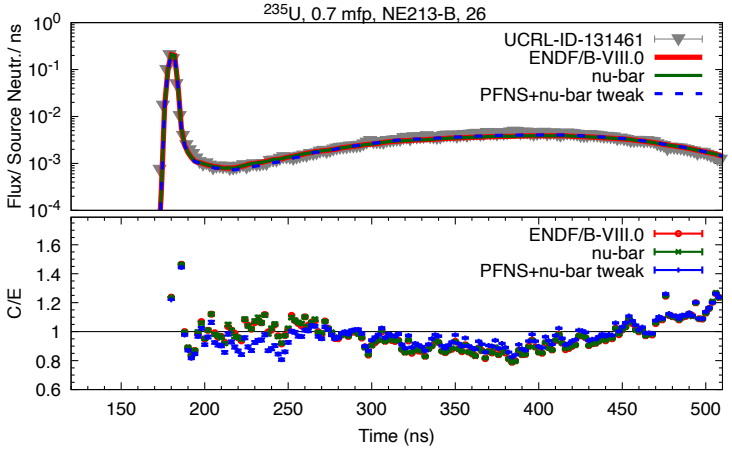
New evaluated ^{235}U nu-bar and PFNS lead to small changes in k_{eff} of a few HEU and IEU MET-FAST experiments.

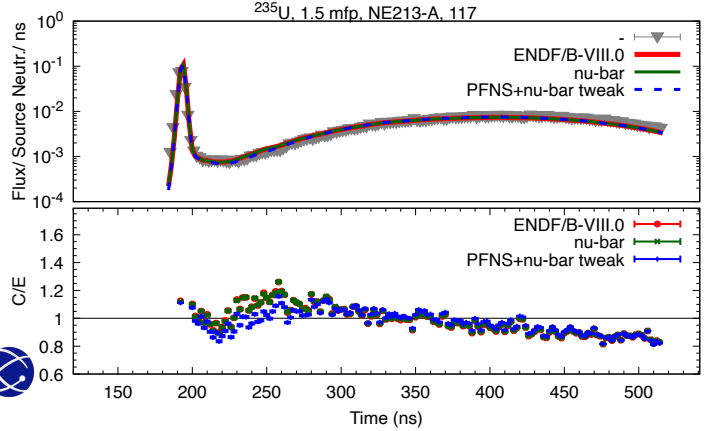
Table II: Simulated and experimental k_{eff} values are compared with each other for ENDF/B-VIII.0, ENDF/B-VIII.0 with the new PFNS for E_{inc}=0.5–30 MeV and ENDF/B-VIII.0 with the new PFNS for E_{inc}=0.5–30 MeV and a tweaked $\overline{\nu}_p$ from Resf. [27, 28]. An abbreviated ICSBEP nomenclature is used to identify the ICSBEP critical assembly [7]. HMF001 is the Godiva assembly, HMF028 is Flattop, IMF1 is Jemima and IMF7 is BigTen.

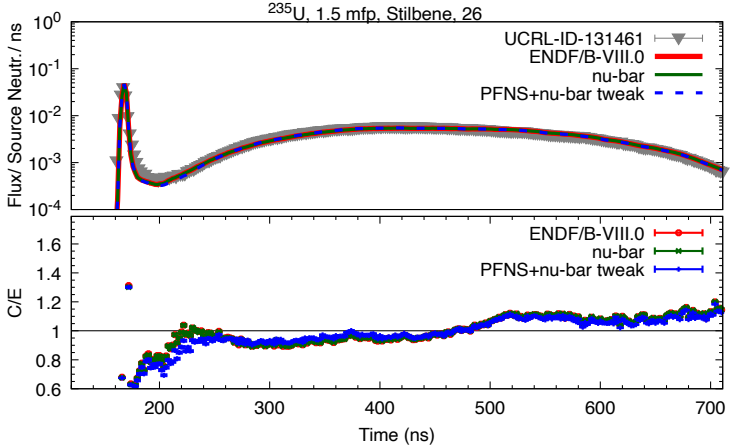
Benchmark	Exp.	Exp. Unc. (pcm)	VIII.0	PFNS	PFNS -VIII.0 (pcm)	$\overline{\nu}$+PFNS	($\overline{\nu}$+PFNS) -VIII.0 (pcm)	MC Unc. (pcm)
HMF001	1	100	1.00016	0.99964	-52	1.00047	31	8
HMF028	1	300	1.00092	1.00052	-40	1.00104	12	9
IMF1.1	0.9988	90	0.99888	0.99859	-29	0.9989	2	9
IMF1.2	0.9988	90	0.99919	0.99871	-48	0.99921	2	9
IMF1.3	0.999	30	0.99824	0.99786	-38	0.99812	-12	9
IMF1.4	0.999	30	0.9992	0.99895	-25	0.99914	-6	9
IMF7d	1.0045	70	1.00433	1.00402	-31	1.00421	-12	7

New evaluated ^{235}U PFNS improves simulated neutron leakage spectra of LLNL pulsed spheres.









New integral exp. mapping out the ^{235}U PFNS are coming, and will be used for validation.

Summary

- Currently in VIII.1$\beta 1$:
  - ^{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.
  - ^{235}U nu-bar including CGMF modeling,
  - ^{235}U PFNS including Chi-Nu data.
- Delivered:
  - ^{238}U nubar including CGMF modeling,
  - ^{238}U Chi-Nu PFNS.

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To-Do:

- Model, exp. UQ, and evaluate ^{238}U PFNS including at higher E_{inc},
- Benchmark ^{238}U PFNS & nu-bar evaluations,
- Get $^{238,240\text{-}242}$Pu nu-bar.

Thank you for your attention!

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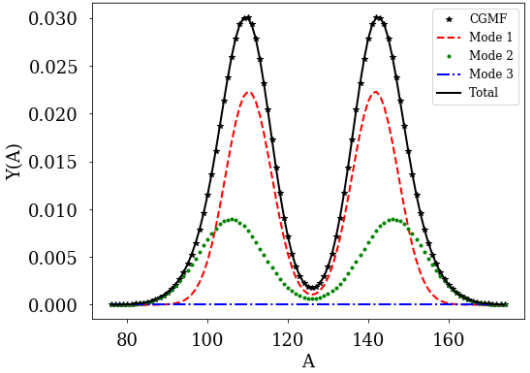
We gratefully acknowledge the support of the Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory.

Back-up

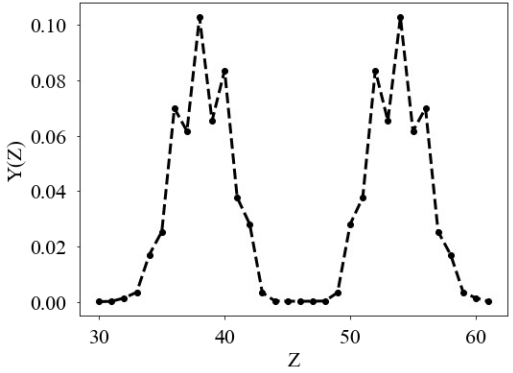
- Modeling
- Experimental UQ

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

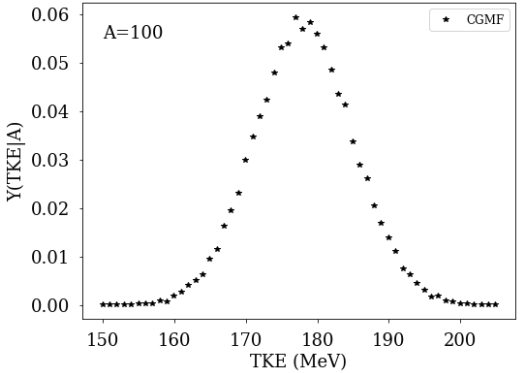
3 Gaussians



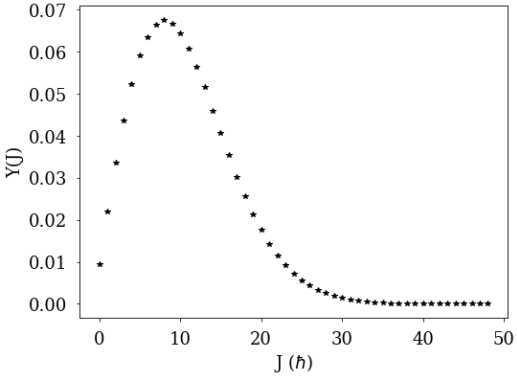
Wahl Systematics



Gaussian per mass



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



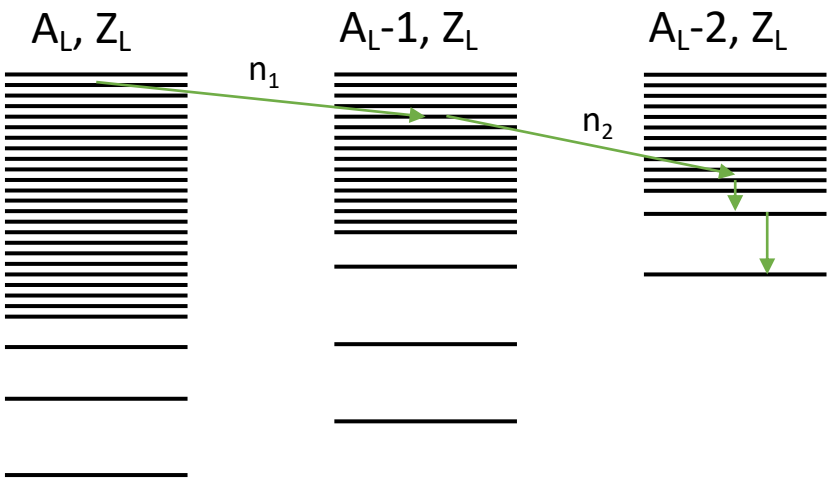
These initial conditions are essentially shared between the two codes – we can utilize optimization from one code for the other.

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

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

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

The Hauser-Feshbach statistical theory is used to de-excite the fission fragments



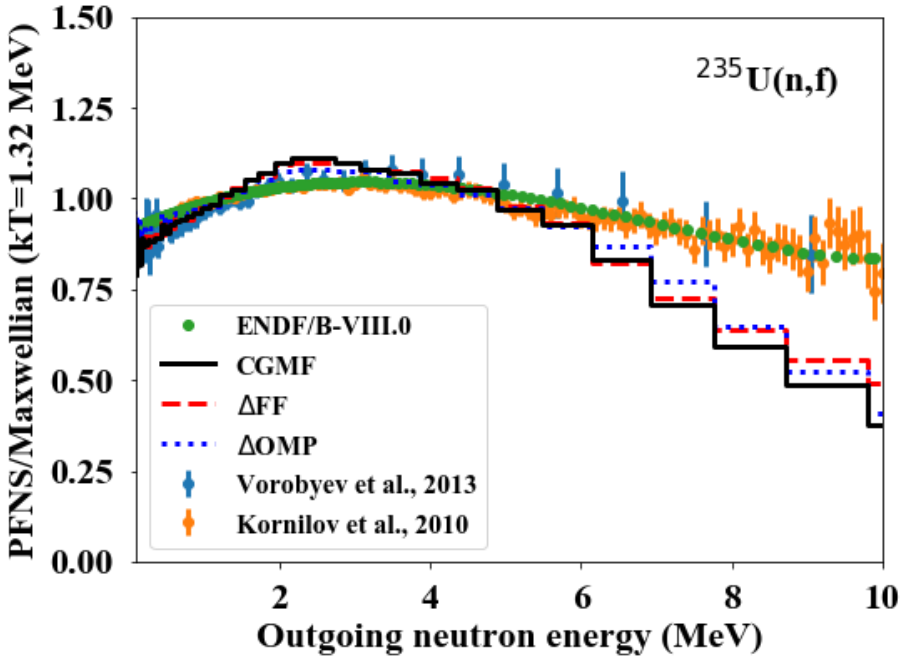
Energy, momentum, spin, and parity are conserved during the decay

Other nuclear information is needed for modeling

- 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.

LA-UR-21-30882

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

PFNS evaluations are still performed using the Los Alamos Model while further studies are ongoing.

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

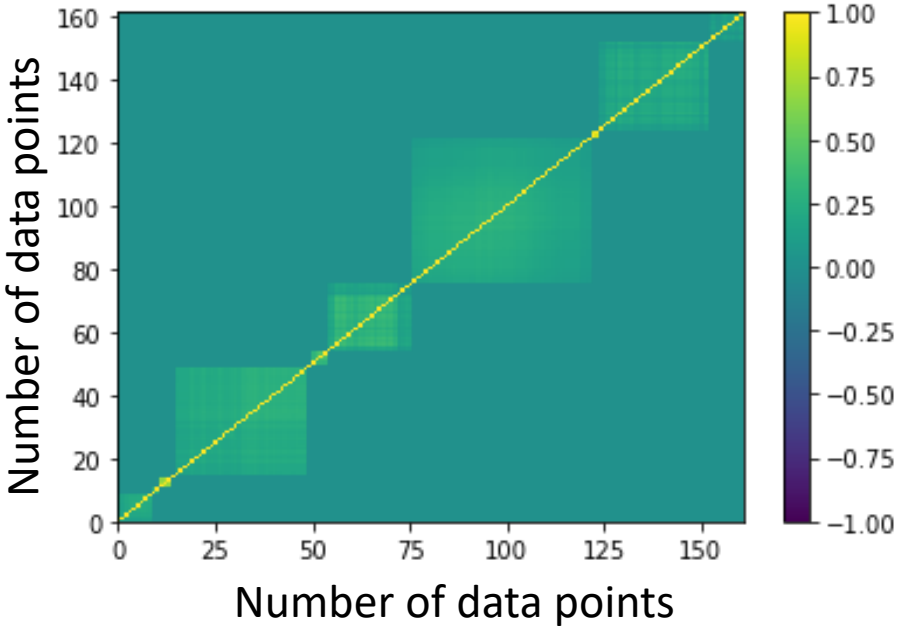
ARIADNE modules:

- 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).



^{238}U nu-bar exp. cov. estimated with *ARIADNE*.