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Producing Evaluation-quality ^{239}Pu Average Prompt Fission Neutron Multiplicities using a Correlated Fission Model

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Abstract. An evaluation of the average prompt fission neutron multiplicity, $\bar{\nu}_p$, of ^{239}Pu(n,f) is shown. This evaluation includes (a) the correlated fission model CGMF, and (b) a detailed analysis of past and recently published experimental data. Using CGMF-calculated $\bar{\nu}_p$ as prior enables to link, through the use of evaluated model input parameters, $\bar{\nu}_p$ to other fission observables such as the prompt fission neutron spectrum (PFNS), pre-neutron emission fission yields as a function of mass, and the average total kinetic energy of the fragments. These evaluated parameters produce realistic predictions of many fission observables, while the evaluated $\bar{\nu}_p$ agrees well ($\chi^2 \approx 1$) with data. Moreover, with the new evaluated $\bar{\nu}_p$, the effective neutron multiplication factor of fast Pu ICSBEP critical assemblies are predicted with a mean bias of 58 pcm compared to 18 pcm with ENDF/B-VIII.0, when paired with a new ^{239}Pu PFNS and fission cross section. Due to these encouraging validation results, the evaluated $\bar{\nu}_p$ is currently part of a release candidate for the ^{239}Pu ENDF/B-VIII.1 file. Hence, a correlated fission model was used for the first time for evaluating $\bar{\nu}_p$ that is of evaluation quality. This is an important step towards consistent evaluations of prompt fission observables.

1 Introduction

Historically, there is little to no consistency between the various types of fission nuclear data in our evaluated libraries [1]. However, we know that these observables are correlated through the fission process that produces all of them. For instance, the energies and multiplicities of prompt neutrons and gamma rays are correlated through the total excitation energy of the fission fragments, but are usually evaluated separately with different types of models or, in some cases, entirely based on experimental data that do not reflect such correlations.

To address these inconsistencies and potential biases that arise from them, correlated fission models have been developed in the last decade. One can, for instance, use the LANL-developed Monte Carlo Hauser-Feshbach statistical decay code CGMF [2] to calculate the prompt emission of neutrons and gamma rays from excited fission fragments, conserving energy, momentum, spin, and parity at each step in the decay. This code ultimately computes the desired average prompt fission neutron multiplicity, $\bar{\nu}_p$, and prompt fission neutron spectrum, PFNS, within the same framework. However, these models do not typically predict $\bar{\nu}_p$ and PFNS to the precision needed for nuclear data evaluations and applications. To this end, experimental data for these observables need to be included in a formal evaluation procedure.

Here, we present the first of such a CGMF-informed evaluation for ^{239}Pu(n,f) $\bar{\nu}_p$. Section 2 briefly summarizes the evaluation input. In Section 3, it is shown that the evaluated ^{239}Pu(n,f) $\bar{\nu}_p$ reproduces experimental data, and that the evaluation also produces results for other fission observables that compare well with experimental data. Moreover, these evaluated data performed well in simulating the effective neutron multiplication factor of fast ICSBEP critical assemblies [3], when combined with recent evaluations of ^{239}Pu(n,f) PFNS and fission cross sections. Section 4 provides a summary, conclusions, and an outlook.

2 Evaluation input

Evaluation procedure

Evaluated data were obtained with the Kalman filter method [4], implemented in the ARIADNE code [5], which uses Bayes' theorem to update prior parameter values and their uncertainties calculated with CGMF, with experimental data and their covariances. Sensitivities of CGMF predicted $\bar{\nu}_p$ to its input parameters link the model parameters space with that of experimental $\bar{\nu}_p$. The evaluated parameters obtained with the Kalman filter are fed back into CGMF to compute the evaluated ^{239}Pu $\bar{\nu}_p$ shown in Fig. 1. Those parameters are also used to predict, at the same time, pre-neutron emission yields as a function of mass, fission fragment total kinetic energy, prompt gamma and neutron observables as shown for a few examples in Fig. 2.

CGMF *input as prior*

CGMF [2] starts by sampling the initial conditions of the fission fragment distributions in mass, charge, total kinetic energy, spin and parity, $Y(A, Z, \mathrm{TKE}, J, \pi)$. These distributions are parametrized and fit to available experimental

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data. Once the initial conditions are sampled, neutrons and γ rays are emitted from the excited fragments using the Hauser-Feshbach statistical theory [6]. The initial conditions of the fission fragments, and the energies and directions of the prompt neutrons and γ rays are collected, which allows for the reconstruction of prompt observables and their correlations.

To fit $\bar{\nu}_p$, we vary the parameters for the mass, total kinetic energy, and spin distributions. These parametrizations are specified for the first-, second-, and third-chance fissioning systems. The fourth-chance fission parameters are not included in the optimization as the fourth-chance channel is less than 2% at 20 MeV incident neutron energy. `CGMF` is run with the default parametrization to calculate the baseline $\bar{\nu}_p$ values, and then sensitivities are calculated by varying each parameter by $\pm 1\%$.

Experimental data

Experimental $\bar{\nu}_p$ selected for the evaluation are shown in Fig. 1. All of these data were extracted from the EXFOR database [7] except for the recently measured ^{239}Pu $\bar{\nu}_p$ by Marini [8] that employ a novel technique. Total uncertainties were all estimated by reading the associated literature, extracting uncertainties from there and EXFOR, complementing uncertainties sources that were missing with templates of expected measurement uncertainties for ^{239}Pu $\bar{\nu}_p$ [9] and using the `ARIADNE` code [5]. No correlations were estimated between experiments except those due to all data being measured as ratios to ^{252}Cf(sf) $\bar{\nu}_p$. Report [10] documents assumptions that were made on uncertainties of individual data sets, as well as providing some reasoning why some data sets were rejected.

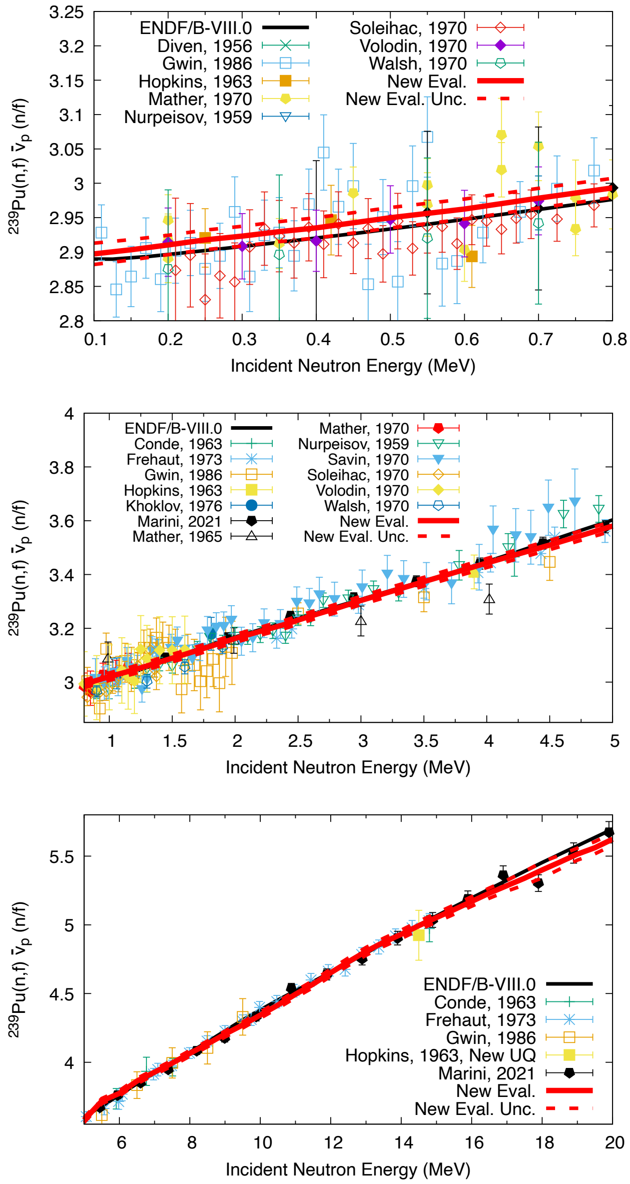

Figure 1. Evaluated ^{239}Pu(n,f) $\bar{\nu}_p$ are compared to ENDF/B-VIII.0 and experimental data that were used for the evaluation.

3 Results and discussion

3.1 Evaluated results

The $\bar{\nu}_p$ in Fig. 1 were computed by `CGMF` using evaluated parameters that resulted from the Kalman filter fit. The evaluated $\bar{\nu}_p$ are close to ENDF/B-VIII.0 [11] from 0.8–4.5, 6–9, and 12–18 MeV. The new evaluation is slightly lower than ENDF/B-VIII.0 from 4.5–5 MeV and slightly higher near 6 MeV, commensurate with second-chance fission structures expected at these energies, and as observed in the `CGMF` prior. A similar effect can be observed from 9–12 MeV due to third-chance fission. These non-linear structures in $\bar{\nu}_p$ are also supported by Marini data [8]. They are not visible in ENDF/B-VIII.0 as past experimental data were too uncertain to capture the effects of second and third-chance fission. At 20 MeV, $\bar{\nu}_p$ from `CGMF` is slightly lower than Marini data, which could be influenced slightly by the inclusion of the fourth-chance parameters in fit. Below 800 keV, the $\bar{\nu}_p$ evaluated with `CGMF` is higher than ENDF/B-VIII.0 but well within the considerable spread of differential experimental data.

3.2 Validation with fission observables and criticality experiments

Validation with fission observables

The evaluated parameters were used to calculate various fission observables, namely: pre-neutron emission fission yields as a function of mass, $Y(A)$, observables related to the total kinetic energy of the fission fragments, and prompt neutron and gamma fission quantities such as the PFNS or the prompt fission gamma spectra. The evaluated parameters lead to calculated $Y(A)$ in reasonable agreement with experimental data in the two upper plots of Fig. 2. The predicted average total kinetic energy as a function of incident energy also agrees with many experimental data up to 5 MeV, then it deviates systematically from the phenomenological model data of Lestone [12]. The mean energy of the PFNS calculated from evaluated parameters is, however, too low by ~20 keV. It is a known model defect that CGMF, and other similar Hauser-Feshbach correlated fission codes, predict the PFNS softer than data indicate. This known issue has yet to be successfully resolved.

Validation with critical assemblies

The validation with regards to fission observables shows that the evaluated parameters obtained by fitting to $\bar{\nu}_p$ experiments are consistent with experimental $Y(A)$ and the average total kinetic energy. Validation with respect to the effective neutron multiplication factor, $k_{\rm eff}$, of ICSBEP critical assemblies [3] tests whether the evaluated $\bar{\nu}_p$ are of sufficient quality to predict criticality experiments.

The effective neutron multiplication factor is highly sensitive to $\bar{\nu}_p$. Changes as depicted in Fig. 1 would change $k_{\rm eff}$ significantly. ENDF/B-VIII.0 has been fine-tuned by hand to $k_{\rm eff}$ of selected ICSBEP critical assemblies to predict them with a low bias. Hence, any large change in $\bar{\nu}_p$ would need to be compensated by tweaking other nuclear data. Here, the changes in $\bar{\nu}_p$ are counterbalanced by using new ^{239}Pu(n,f) PFNS and fission cross sections that differ from ENDF/B-VIII.0 due to re-examination of past data, and inclusion of recent high-precision experimental data [13–16].

If one uses this new ^{239}Pu fission source term, one obtains simulated over experimental (C/E) values for $k_{\rm eff}$ plutonium metal fast ICSBEP assemblies shown in Fig. 3 with a mean bias of 58 pcm, while one gets 18 pcm with ENDF/B-VIII.0. One should, however, consider that no tweaks were undertaken on any of the new data, indicating that the new physics from CGMF, and high-precision experimental data lead to evaluated data that as a whole describe $k_{\rm eff}$ reasonably well, while improving the consistency among evaluated fission observables.

4 Summary, conclusions and outlook

An evaluation of the ^{239}Pu average prompt fission neutron multiplicity, $\bar{\nu}_p$, was undertaken that not only includes new high-precision experimental data and a detailed re-assessment of experimental uncertainties of past data, but also brings in the correlated fission model CGMF. Due to this new model and new high-precision experimental data, the evaluated $\bar{\nu}_p$ clearly shows structures commensurate with second and third-chance fission while being close to ENDF/B-VIII.0 for other energies. Moreover, one can use the evaluated parameters of CGMF to predict correlated fission quantities that compare favorably with available data, e.g., on $Y(A)$, the average total kinetic energy, *etc.* The evaluated parameters and $\bar{\nu}_p$ also perform well in predicting $k_{\rm eff}$ of various ICSBEP critical assemblies when paired with the newest PFNS and $(n$,f) cross section that in turn include new high-precision experimental data, and re-assessments of uncertainties of past data. Due to that, the combination of $\bar{\nu}_p$, PFNS, and $(n$,f) cross sections is currently part of an ENDF/B-VIII.0 release candidate. This shows that the evaluated $\bar{\nu}_p$ obtained with CGMF is of evaluation quality. A final, and more detailed, documentation

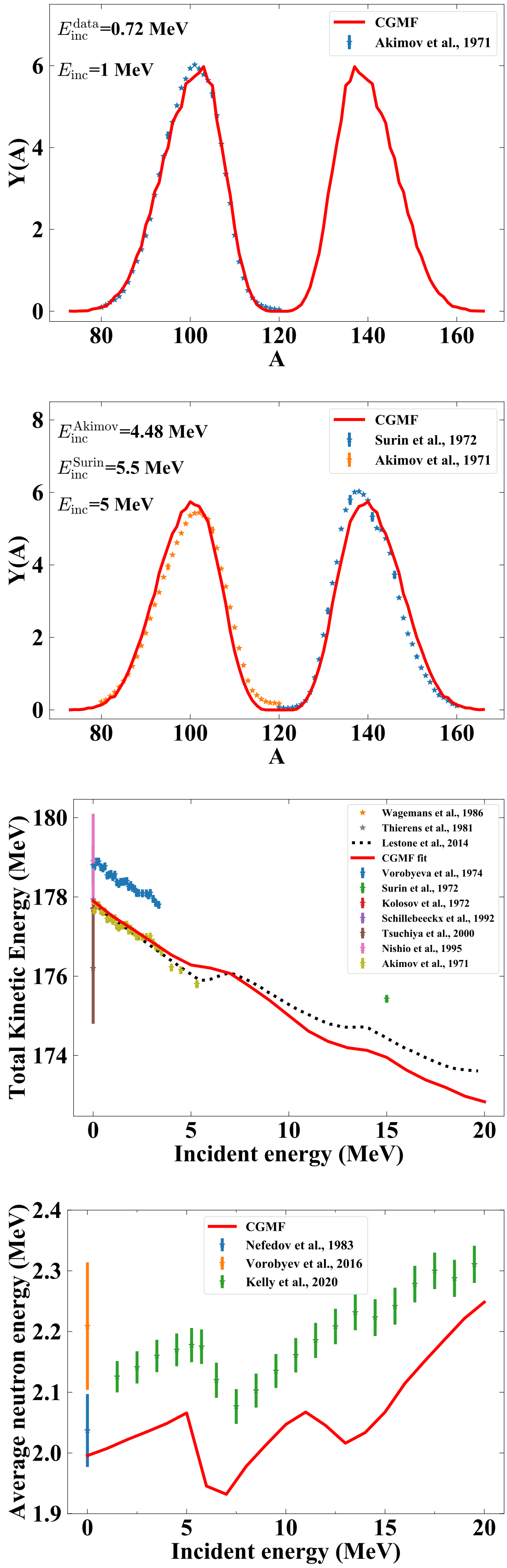

Figure 2. ^{239}Pu(n,f) $Y(A)$, the average total kinetic energy as a function of incident energy, and the mean energy of the PFNS are shown as predicted from CGMF using evaluated parameters. They are compared to experimental data of the same observable.

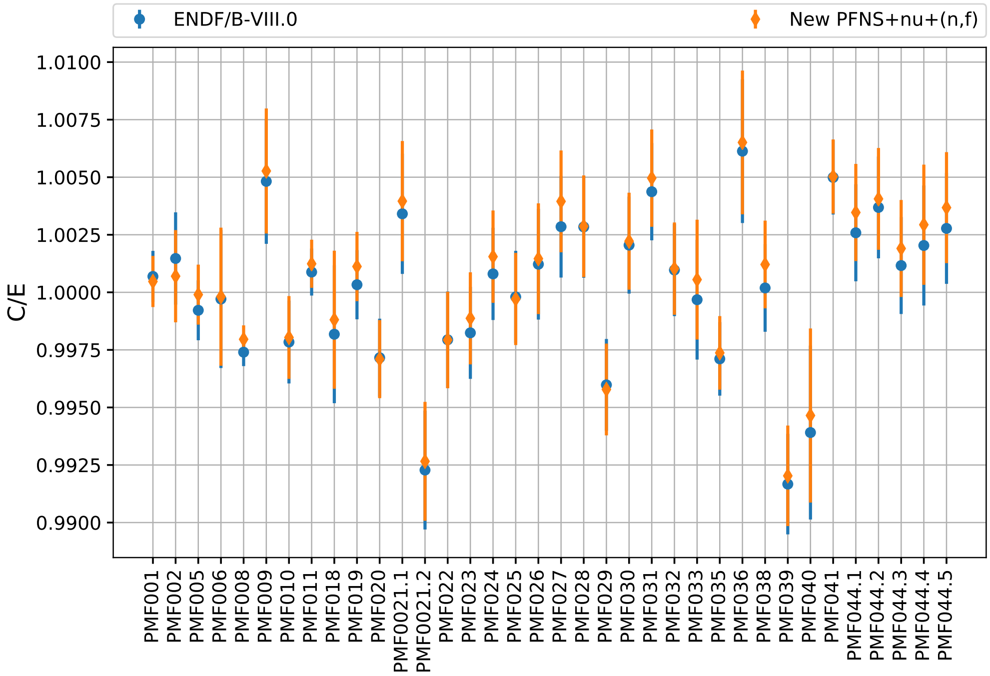

Figure 3. Simulated, C, criticality values of ICSBEP critical assemblies are shown in ratio to experimental values, E, considering total uncertainties on C/E. A short-hand notation is used to identify the ICSBEP critical assemblies [3].

of the combined evaluation work on $\bar{\nu}_p$, PFNS, and (n,f) cross sections is published in Ref. [17].

This demonstration that CGMF can produce evaluation quality $\bar{\nu}_p$ consistent with reasonable $Y(A)$, and average total kinetic energy is an important step towards evaluating fission quantities consistently with each other. One stumbling block, however, is a known model defect in predicting the PFNS with CGMF, which are still too soft compared to experimental data. Hence, modeling efforts will be focused in the future on improving the PFNS description in CGMF, while the code will be used for evaluations of ^{233,235,238}U and Pu minor isotopes in the near future.

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