# Covariance generation for the prompt neutron multiplicity of $^{239}$Pu including the (n,$\gamma$f) process

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**Abstract.** Fission cross section of $^{239}$Pu can be seen as a sum of the "immediate" fission and "two-step" (n,$\gamma$f) reactions. In the Resolved Resonance Range of the reaction cross sections, the contribution of the (n,$\gamma$f) process has an impact on the determination of the partial widths magnitude involved in the Reich-Moore approximation of the R-matrix theory. The present work aims to investigate this impact by using the CONRAD code and the partial width $\Gamma_{\gamma f}$ for the (n,$\gamma$f) reaction calculated by Lynn et al. [1]. A special attention will be paid to the covariance matrix obtained on $\nu_p$.

## 1 Introduction

When a compound system is formed in an excited state by absorbing a low-energy neutron on a target nucleus, it may decay from the excited stated by neutron or $\gamma$-ray emission, or by fission. In fission reactions, depending on the time at which neutrons are emitted, they can be called *prompt* or *delayed* neutrons. If a $\gamma$-ray is emitted before fission, then the available excitation energy to the fission fragment is lower, and less prompt neutrons are emitted.

A one-dimensional description of the fission process was described in [2], as a double-humped potential barrier expressed as a function of the compound nucleus deformation, where the two wells are populated by energy states through which fission may occur. In the first well of this fission barrier, two-step fission reactions are related, in first approximation, to dipole electric (E1) and magnetic (M1) transitions between states [1].

The investigation of the two-step (n,$\gamma$f) process has been developed during the last sixty years, since in 1959 E. Lynn estimated the $\Gamma_{\gamma f}$ width for the (n,$\gamma$f) reaction. In 1988, one of these studies performed by E. Fort [3], treated of the evaluation of $\nu_p$ for $^{239}$Pu. From these background studies, a new description of the prompt-neutron multiplicity for neutron-induced reactions on $^{239}$Pu has been provided in this work, through the analysis of a set of experimental data using the CONRAD[1] code (COde for Nuclear Reaction Analysis and Data Assimilation)[11], taking into the calculations the partial cross sections of the different channels, and the immediate and the two-step fission reactions for the total fission cross section. Preliminary results of this work, obtained by applying the method to two types of description of the experimental data (averaged and pointwise), were presented in [4]. The results here presented correspond to the most accurate treatment of the data.

The calculation of covariances between the nuclear model parameters using integral data assimilation methods may lead to extremely long run times and, the estimation of large covariance and precision matrices via Monte Carlo techniques become difficult due to the dimensionality [5]. This problem can be solved using latent-parameter models, consisting in the calculation of cross-covariance matrices between Gaussian distributed parameters of the neutron-induced reaction models, by introducing variance penalty terms [6]. A variance penalty-based approach has been used in this work to calculate the covariance matrix for $^{239}$Pu.

## 2 Two-step (n,$\gamma$f) process modeling in the RRR

The phenomenological formalism used to express the competition between the two-step and the immediate fission process in the production of prompt neutrons for $^{239}$Pu, was described in [3] by the next formula, since two spins ($J^\pi$=$0^+$ and $J^\pi$=$1^+$) and two phenomena are involved:

$$\upsilon_p \approx \sum_{J^\pi} \nu^{J^\pi} P^{J^\pi}(E_n) \quad (1)$$

where:

$$P^{J^\pi}(E_n) = \frac{\sigma^{J^\pi}_{(n,f)}(E_n) + \sigma^{J^\pi}_{(n,\gamma f)}(E_n)}{\sigma_{ftot}(E_n)} \quad (2)$$

The $^{239}$Pu(n,f) total cross section can be written, indistinctly for spin-parity, as:

$$\sigma_{ftot}(E_n) = \sigma_{(n,f)}(E_n) + \sigma_{(n,\gamma f)}(E_n) \quad (3)$$

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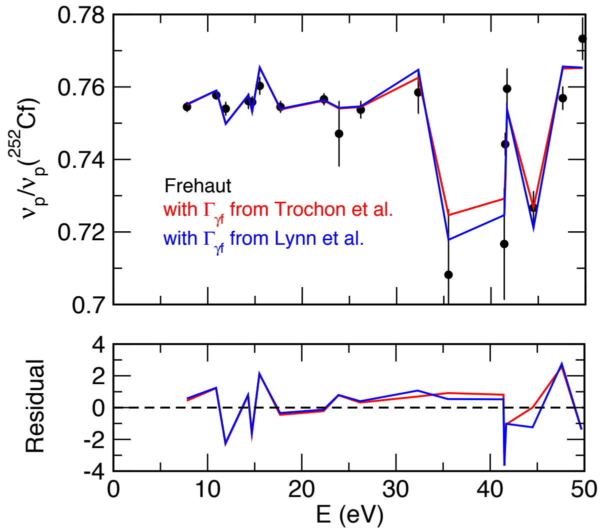


**Figure 1.** Comparison between the results obtained from the CONRAD fit to the experimental data from Fréhaut [8] up to 50 eV, using the values of $\Gamma^{J^\pi}_{\gamma f}$ provided by Trochon et al. [13] and Lynn et al. [1].

where the two-step fission cross section may be expressed as:

$$\sigma^{J^\pi}_{(n,\gamma f)}(E_n) = \sigma^{J^\pi}_{\gamma}(E_n) \cdot \frac{\Gamma^{J^\pi}_{\gamma f}}{\Gamma^{J^\pi}_{\gamma}} \quad (4)$$

To perform the calculations in the Reich-Moore approximation of the R-Matrix Theory, the partial fission widths need to be known. In this work, three immediate fission channels have been considered, as explained in [4], two for $J^\pi = 0^+$ with partial fission widths $\Gamma_{1f}(0^+)$ and $\Gamma_{2f}(0^+)$ and one for $J^\pi = 1^+$, with partial fission width $\Gamma_f(1^+)$ [7]. In the two-step fission process, only two $\gamma$-fission channels have been considered, with partial fission widths $\Gamma_{\gamma f}(0^+)$ and $\Gamma_{\gamma f}(1^+)$, and the second partial width for $J^\pi = 0^+$ has been considered negligible, since (n,$\gamma$f) width fluctuations are negligible.

### 2.1 CONRAD resonance analysis and results

The experimental datasets available in the EXFOR database of the prompt neutron multiplicity for $^{239}$Pu, are those measured by Fréhaut [8] and Gwin [9, 10] with a given normalization.

An accurate evaluation must include the (n,$\gamma$f) channel for $J^\pi = 1^+$ resonances [1], while the current one only treats these resonances as decaying through immediate fission. For this purpose a new calculation has been performed using the R-Matrix code CONRAD. Total and partial cross sections, and neutron multiplicities have been analyzed together. The partial fission widths for immediate fission have been extracted from the JEFF-3.3 evaluation, and the partial fission widths for the two-step fission reactions have been taken from the work of Trochon et al.: $\Gamma_{\gamma f}(J^\pi = 0^+) = 7.3$ meV and $\Gamma_{\gamma f}(J^\pi = 1^+) = 4.2$ meV, or Lynn et al.: $\Gamma_{\gamma f}(J^\pi = 0^+) = 1.5$ meV and $\Gamma_{\gamma f}(J^\pi = 1^+) = 2.29$ meV, and the results have been compared. The s-wave average radiative width ($<\Gamma_\gamma>$) = 43 ± 4 meV has been taken from Mughabghab [12].

**Table 1.** Output parameters obtained from the fit to the $\nu_p$ experimental data.

| Parameter | With $\Gamma_{\gamma f}$ from [13] | With $\Gamma_{\gamma f}$ from [1] |
|---|---|---|
| $<\nu_{n\gamma f}>$ | 2.60 ± 0.02 | 2.41 ± 0.03 |
| $<\nu_0>$ | 2.897 ± 0.002 | 2.894 ± 0.002 |
| $<\nu_1>$ | 2.874 ± 0.002 | 2.873 ± 0.002 |
| $N_{Frehaut}$ | 0.9963 ± 0.0007 | 0.9965 ± 0.0007 |

The parameters used to fit the data below 50 eV using CONRAD are the $\nu_{n\gamma f}$, $\nu_0$, $\nu_1$, and the normalization. Results of present fit using both sets of values for $\Gamma_{\gamma f}$ from [1, 13], are given in Figure1 and Table1. It shows that the use of both values for $\Gamma_{\gamma f}$ provides similar results, as it is balanced by fitting $<\nu_{n\gamma f}>$. However the value 2.60 obtained for the parameter $<\nu_{n\gamma f}>$ seems to be more realistic than the value 2.41 from a physics ground.

### 2.2 Calculations up to 500 eV

Below 50 eV the data from Fréhaut and Gwin are well described by the equations, showing that the spin contribution can reproduce the experimental data below 25 eV, while above this energy the dips are reproduced using the $\nu_{n\gamma f}$ contribution.

However at higher energies, the large dispersion of the experimental data (1.2%) prevents a good description, see Figure 2. New experimental data with lower statistical uncertainties are needed in this higher energy region.

## 3 Covariance matrix

The neutron cross section evaluation provides a phenomenological description of a nuclear reaction with a large number of parameters, dealing to an optimization problem because all of the model parameter covariances cannot be simultaneously estimated from well-defined sets of experimental data. This situation can be simplified dividing the model parameter sequence into blocks of variables, which uncertainties can be propagated through fixed-order sequential data assimilation procedures. Those are "observable" variables, that can be directly determined from the experimental data, "latent" variables, that may define redundant parameters or hidden variables which cannot be directly observed, and "nuisance" variables, that correspond to physical realities with fundamental properties for assessing reliable model parameters.

Considering only the uncertainty propagation of the observable and latent parameters, the covariance matrix $\Sigma$ between model parameters $\mu$ can be expressed as:

$$\mu = \begin{pmatrix} x \\ \theta \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \quad (5)$$

where $x = (x_1 ... x_n)^T$ are the observable parameters, and $\theta = (\theta_1 ... \theta_m)^T$ are the latent parameters.

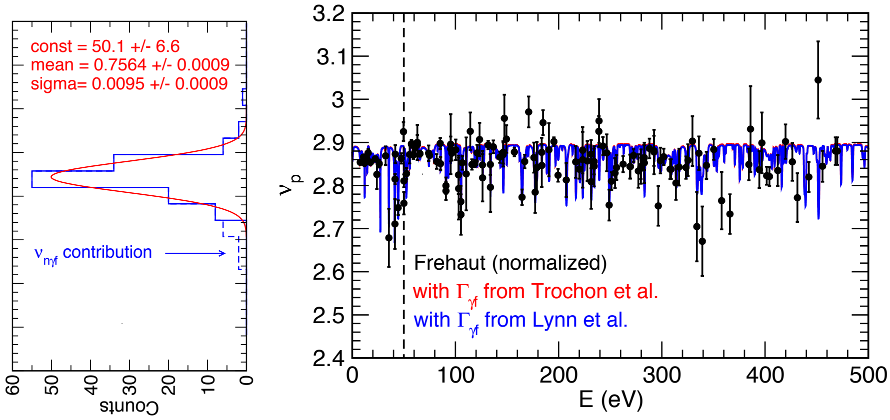


**Figure 2.** Comparison between the $\nu_p$ results obtained up to 500 eV using $\Gamma_{\gamma f}^{J^\pi}$ from Trochon et al. and Lynn et al., and the normalized data from Fréhaut (right panel). The $\nu_p$ histogram of the data from Fréhaut has been fitted to a gaussian distribution (left panel), showing a dispersion of 1.2%.

### 3.1 Variance Penalty-based approach

In this approach, the parameter column vector $\mu$ is divided into an n-dimensional column vector x containing “passive" variables and a m-dimensional column vector $\theta$ containing “active" variables. Hence passive variables are equivalent to observable parameters, and active variables to latent parameters. The observable parameters are of special interest for the neutron cross section evaluation, and the latent variables have known variances and covariances.

A Monte Carlo algorithm based on a least-squares fitting procedure has been used to calculate the elements of the full covariance matrix from Equation 5, that results in:

$$\begin{cases} \Sigma_{11} \simeq M_x + M_x^{\theta} \\ \Sigma_{22} = M_{x,\theta} \\ \Sigma_{12} = M_{\theta} \end{cases}$$

where $M_x$ is the covariance matrix between the best-fitted values of the observable variables, and $M_\theta$ is the covariance matrix between the latent variables.

The Zero Variance Penalty Condition is achieved when the variance of the passive variables is equal to the variance of the active variables, being used to simplify the calculation of the matrices $M_x^\theta$ and $M_{x,\theta}$ of the full covariance matrix elements. It becomes:

$$\begin{cases} \Sigma_{11} = M_x + (G_x^T G_x)^{-1} G_x^T G_\theta M_\theta G_\theta^T G_x (G_x^T G_x)^{-1} \\ \Sigma_{12} = -(G_x^T G_x)^{-1} G_x^T G_\theta M_\theta \\ \Sigma_{22} = M_\theta \end{cases}$$

For more details check reference [5].

### 3.2 Covariance matrix results

In this work, the latent variables are the resonance parameters from JEFF-3.3, which are used to calculate the neutron cross sections and associated uncertainties.

The prompt neutron multiplicity ($\nu_p$) and uncertainties obtained using this method with the experimental data from Fréhaut [8] and Gwin [9, 10], are shown in Figure 3. Present values obtained for the prompt and the delay neutron multiplicities at 25.3 meV are 2.872(12) and 0.0065(10) respectively. Hence, a total neutron multiplicity at thermal energy of 2.879(12) is obtained, in excellent agreement with the standard value of 2.878(13).

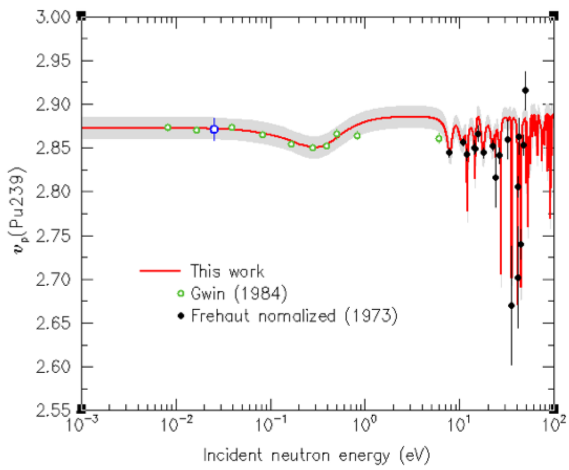


**Figure 3.** Results for the $^{239}$Pu prompt neutron multiplicity.

The results obtained for the covariance matrix of $\nu_p$(E) are shown in Figure 4.

## 4 Conclusions and perspectives

A new evaluation of the prompt neutron multiplicities for $^{239}$Pu(n,f) taking into account both, the “immediate” and the “two-step” contributions to the total fission cross section, is summarized in this paper. The CONRAD code has been used to perform a multiple analysis of the total and partial cross sections, as well as the total and prompt neutron multiplicities. According to the prompt neutron

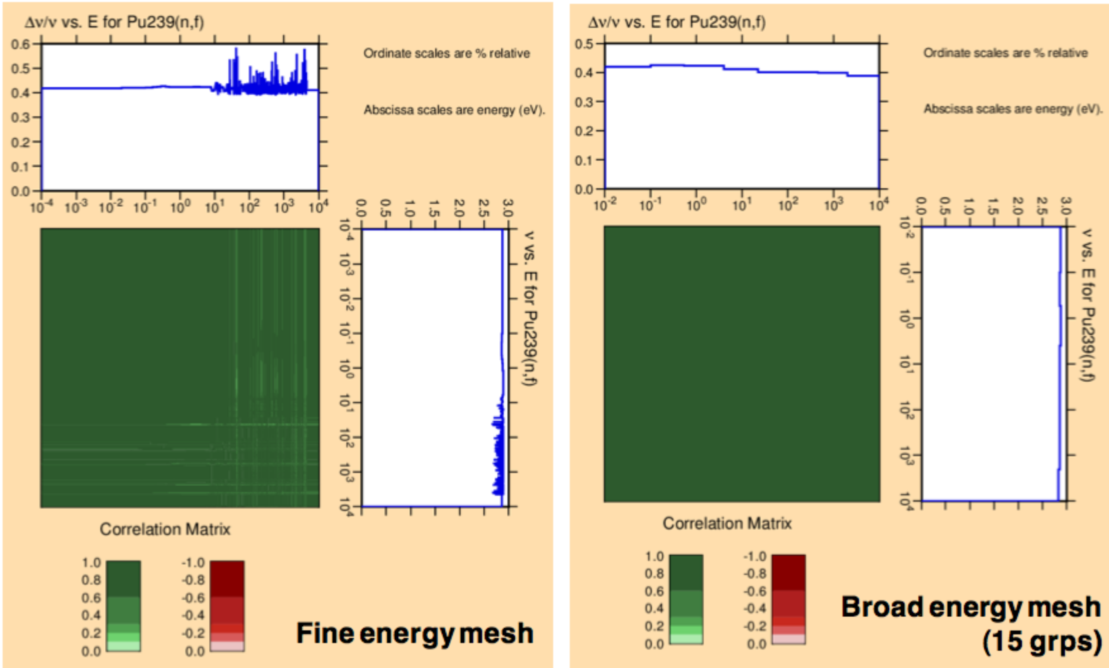


**Figure 4.** Covariance matrix for the $^{239}$Pu prompt neutron multiplicity using a fine and a broad energy mesh.

multiplicity, two sets of experimental data, measured by Fréhaut and Gwin, are provided at low energies in the EXFOR database. A normalization factor must be assigned to each of the two data sets. The $\nu_p$ experimental data have been fitted in order to calculate $\nu_{n\gamma f}$, $\nu_0$, $\nu_1$, and the normalization parameter. In order to perform the calculations, the resonance parameters for the immediate fission have been extracted from the JEFF-3.3 evaluation, and the two proposed values for the $\Gamma_{\gamma f}$ parameter [1, 13] have been tested, both giving similar results but a lower $<\nu_{n\gamma f}>$ using the recommendation from [1].

Above 50 eV, the large dispersion (1.2%) of the data from Fréhaut does not allow to reproduce them. Hence new experimental data are highly demanded in this energy region. For this purpose, new measurements of the $\nu_p$ for $^{239}$Pu are in progress at JRC-Geel.

A variance penalty-based approach applying the zero variance penalty condition [5], has been applied to calculate the prompt neutron multiplicity covariance matrix for $^{239}$Pu(n,f). The total neutron multiplicity obtained at thermal energy using this approach is 2.879(12), in excellent agreement with the value of 2.878(13) that is recommended on “the standards".

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