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A methodology for the intercomparison of nuclear fission codes using TALYS

Andrea Mattera, Ali Al-Adili, Mattias Lantz, and Stephan Pomp[a], Vasileios Rakopoulos, and Andreas Solders

Uppsala University, Box 516, 75120 Uppsala, Sweden

Abstract. Codes for the calculation of fission observables are frequently used to describe experimentally observed phenomena as well as provide predictions in cases where measurements are missing. Assumptions in the models, and tuning of parameters within the codes, often result in a good reproduction of experimental data. In this work we propose a methodology, coded in the newly developed program DELFIN (De-Excitation of FIssion fragmeNts), that can be used to compare some of the assumptions of the various models. Our code makes use of the fission fragments information after scission and processes them in an independent and consistent fashion to obtain measurable fission observables (such as $\bar{\nu}(A)$ distributions and Isomeric Fission Yield ratios).

All the available information from the models, such as fragments' excitation energies, spin distributions and yields are provided as input to DELFIN that uses the nuclear reaction code TALYS to handle the de-excitation of the fission fragments. In this way we decouple the fragments relaxation from the actual fission models.

We report here the first results of a comparison carried out on the GEF, Point-by-Point and FREYA models for thermal fission of ^{235}U and ^{239}Pu and spontaneous fission of ^{252}Cf.

1. Introduction

In this work, we propose a way of comparing the many available fission codes in the description of observables that can be fitted to experimental data, such as isomeric yield ratios and prompt neutron emission distributions $\bar{\nu}(A)$. This is done in order to get a closer look *under the hood* of the models, trying to distinguish between the physics assumptions (e.g. the sorting of excitation energy E^* between the two fission fragments (FF)) and what is the process of extracting the observables (e.g. the de-excitation of the FF to obtain $\bar{\nu}(A)$).

In particular, we believe that eliminating any variability in the way the final observables are extracted could help focus on the models' assumptions and possible shortcomings. This can be achieved using the quantities defined "at scission" by the fission model and introducing a transparent way of handling the fragments' de-excitation consistent for all fission codes. We propose the TALYS reaction code [1] as a tool to carry out the de-excitation of the FF and extract the desired observables.

The preparation of the TALYS inputs from the E^* distributions calculated by the models under test and the extraction of the final observables have been bundled in a single code: DELFIN (De-Excitation of FIssion fragmeNts).

The work was developed in various steps aimed at developing and validating the methodology. The first phase (ⓐ1 and ⓑ1 in Fig. 1) was carried out making extensive use of the GEF code [2] to test DELFIN, whose details will be discussed in Sect. 2. Some of the first results of the actual comparison of different models (step ② in Fig. 1) will be shown in Sect. 3.

2. Methodology

The principle we followed in the development of DELFIN is transparency: no arbitrary assumptions have been made on any quantity needed in the calculations. The process is completely reproducible and – at this stage – the default values of the physics parameters were not modified in the TALYS code. If a value needed for the calculation is not directly provided by the fission models themselves (e.g. FF yields, Z(A) distributions, ...) we turn to well-known systematics.

DELFIN can read input files with the results from any fission model providing information on the FF: the excitation energy $E^*(A)$ and, if available, the spin J. For the de-excitation of FF we use the nuclear reaction code TALYS-1.8.

Since its launch in 2004, TALYS has been increasingly used in fundamental as well as applied nuclear physics and is at the core of the TALYS Evaluated Nuclear Data Library TENDL [3]. One of the features of the TALYS code is the possibility to run de-excitation of a compound nucleus using the embedded Hauser-Feshbach model. This can be done by providing TALYS with a matrix of E^*,J distributions of the compound nucleus (the primary FF, in our case).

DELFIN automatically runs a TALYS calculation for each FF. Depending on the quantity to be extracted, the output of several TALYS runs may be combined. The results are then weighed using the FF yields.

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[a] e-mail: `stephan.pomp@physics.uu.se`

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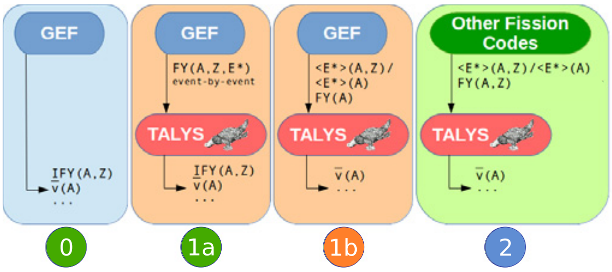

Figure 1. Schematics of the outlined plan for the development of a methodology to compare nuclear fission codes. The main idea is to detach the actual fission modeling from the de-excitation of the FF. This latter is handled in a consistent way using the TALYS reaction code.

2.1. Overview of the DELFIN code

Prompt neutron emission distributions, $\bar{\nu}(A)$, are one of the first quantities studied in this work. We considered it as a good starting point to have an overall perception of the capabilities of the method, since $\bar{\nu}$ is a quantity very tightly related to the excitation energy provided as input and is considered experimentally well known.

In order to obtain $\bar{\nu}(A)$, DELFIN runs a TALYS calculation for each of the FF in an isobaric chain i with mass A_i. The number of prompt neutron $\bar{\nu}(A_i)$ is obtained by averaging the number of neutrons emitted by each FF in the chain. DELFIN automatically repeats the procedure for all isobaric chains i. Information on the relative yield of each fragment, $Y(Z|A_i)$, is needed. If the mass yields $FY(A_i)$ of the isobaric chains are also known, DELFIN provides the total average neutron multiplicity $\bar{\nu}$.

We also used DELFIN to extract other quantities from the TALYS output (such as Isomeric Yield Ratios), but here we only report the results on $\bar{\nu}(A)$.

2.2. Validation of the methodology using the GEF code

The first step in the development of the methodology was to understand what parameters of the fission models would mostly affect the desired quantities to be extracted. In particular, a test was performed to evaluate how much the input could be simplified (i.e. how little information would be required from the fission model, for instance by taking the average E^* instead of the whole distribution) before the results would start deviating considerably from the original calculation.

The GEF code proved to be a valuable tool in this phase, for its ability to provide extensive information on the FF on an event-by-event basis. The validation of the methodology was then performed comparing the results of DELFIN to which - at each step - some information from the primary FF was removed. The result of this sequence of calculations for the $\bar{\nu}(A)$ of $^{235}U(n_{th},f)$ is shown in Fig. 2, where:

(a) **GEF | E_distrib(A,Z)** is the $\bar{\nu}(A)$ distribution obtained running the standalone GEF code.

(b) **DELFIN | E_distrib(A,Z)** is the $\bar{\nu}(A)$ distribution extracted from a calculation in which the complete E^* distribution is provided as input. A DELFIN calculation is run using the yields provided by the GEF code.

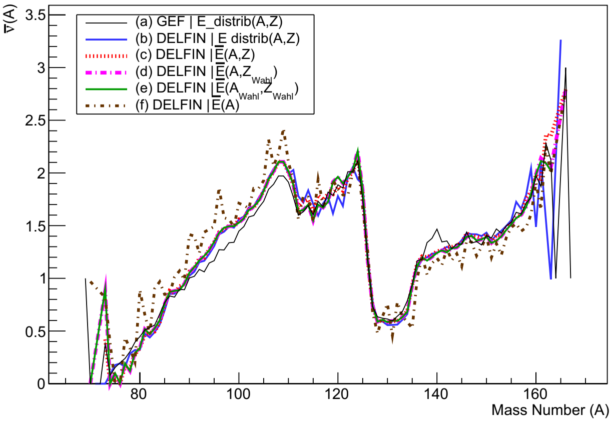

Figure 2. Validation of the methodology using the GEF code for the reaction $^{235}U + n_{th}$. Details of all calculations are discussed in the text.

(c) **DELFIN | $\bar{E}$(A,Z)** as the previous step, but instead of the entire E^* distribution, only the average of the distribution is used as input parameter.

(d) **DELFIN | $\bar{E}$(A,Z_{Wahl})** as the previous step, but instead of the FY(Z,A) from GEF, for each A chain, the Wahl systematics [4] is used to determine the relative contribution of each isobar in terms of yield. The total mass chain yield is obtained from GEF.

(e) **DELFIN | $\bar{E}$(A_{Wahl},Z_{Wahl})** as the previous step, but both Z and A yields are obtained from the Wahl systematics. This step allows us to justify the use of a simple $E^*(A)$ distribution, without any information provided by the fission model on the Z of the FF.

(f) **DELFIN | $\bar{E}$(A)** in this case DELFIN runs only one TALYS calculation for each isobaric chain A. The charge of the FF is selected based the Unchanged Charge Distribution (UCD) model. Comparing this curve with the curve in case (b), we concluded that this simplification is too crude to produce acceptable results for our study.

This extensive testing of the methodology, presented in Fig. 2, demonstrated that the use of the average excitation energy for the isobaric chain (cases (c) to (e)) gives results that are in very good agreement with those obtained using the whole $E^*_{distrib}(A,Z)$ distribution, provided that several FF in a mass chain are included in the calculation. In the calculation of $\bar{\nu}(A)$ in case (e), all the isobars for which Wahl's systematics predicts a non-zero yield were included in the averaging process. On the other hand, using only one isotope per mass chain (case (f)) produces very staggered data points that do not reproduce the original $\bar{\nu}(A)$ distribution.

In addition to this, the generally good agreement between TALYS' de-excitation and GEF standalone, reassured us on the choice of model parameters for the FF used in the TALYS reaction code.

A word of caution: E_{rot}

The GEF code calculates the excitation energy E^* available at scission for each of the FF as the sum of different contributions:

$$E^*_{FF} = E_{int} + \frac{E_{coll}}{2} + E_{def} + E_{rot} \qquad (1)$$

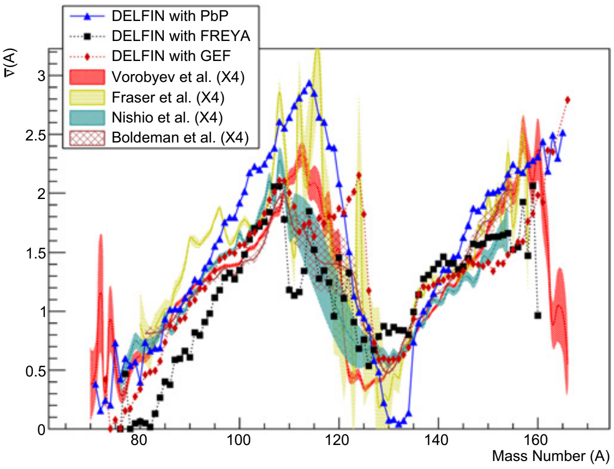

Figure 3. ^{235}U + n$_{th}$ ν(A) distributions as obtained by DELFIN using GEF (--♦--), PbP (–▲–) and FREYA(FF) (--■--) are compared to experimental data [7–10].

where E$_{int}$ is the intrinsic excitation energy, E$_{coll}$ is the total collective energy that is shared equally between the two FF (hence the $\frac{1}{2}$ factor), E$_{def}$ is the deformation energy of the nascent fragment at scission and E$_{rot}$ is its rotation energy. After scission, the FF relax to a less deformed shape and the deformation energy E$_{def}$ will convert into intrinsic energy [2,5].

The rotation energy E$_{rot}$, however, will not be available to the FF statistical excitation and thus for de-excitation through neutron emission. In order to take this into account, the original event-by-event output of the GEF code that calculates E* from Eq. (1) was modified and E$_{rot}$ was subtracted before the excitation energy distributions were used in DELFIN.

3. First results

At this stage, we seek a comparison of the codes with each other as well as with experimental data. We then focused our attention to the most studied reactions for which experimental data are available: ^{235}U(n,f), ^{239}Pu(n,f) and ^{252}Cf(sf).

3.1. ^{235}U(n$_{th}$,f)

The first case we analyzed was neutron induced fission of ^{235}U for which E*(A) are published for several codes. The Point-by-Point (PbP) model [5], calculations with the FREYA code[1] [6] and the GEF output were all processed and compared: the results are shown in Fig. 3 compared to a sample of available experimental data [7–10].

For the sets of E*(A) from FREYA and PbP, information on the FF yields was not provided and was obtained from the Wahl systematics.

3.2. ^{239}Pu(n$_{th}$,f)

The results for neutron-induced fission of ^{239}Pu are shown in Fig. 4 for the GEF and FREYA codes[1], where the calculations from the standalone versions of the codes are compared to those processed using DELFIN. Also in this case, the FF yields for the FREYA calculation were obtained from the Wahl systematics.

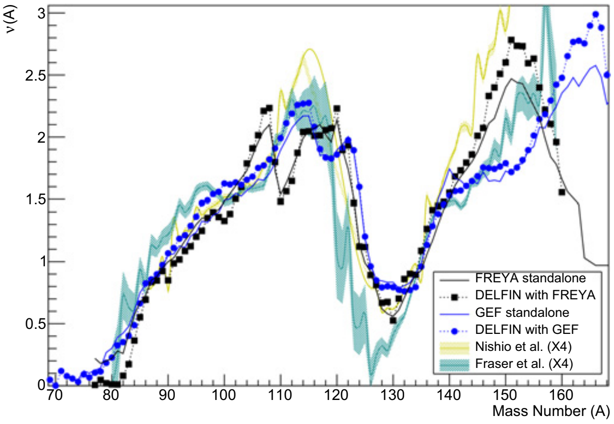

Figure 4. ^{239}Pu+n$_{th}$ $\bar{\nu}$(A) distributions as obtained by DELFIN using FREYA (--■--) and GEF (--●--), compared to the results from FREYA (—) and GEF (—) standalone codes and to experimental data [10,11].

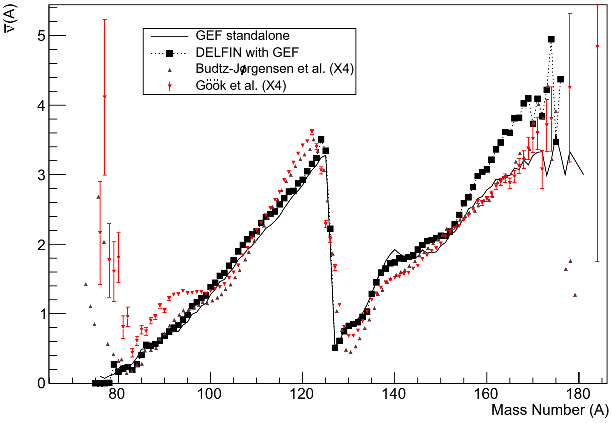

Figure 5. ^{252}Cf SF $\bar{\nu}$(A) distribution as obtained by DELFIN using GEF (--■--), compared to the GEF standalone code (—) and experimental data [12,13].

With respect to the case of thermal fission of ^{235}U shown in Fig. 3, the codes seem to be in better agreement with each other as well as with experimental data for A<140.

3.3. ^{252}Cf(sf)

The calculated $\bar{\nu}$(A) for spontaneous fission of ^{252}Cf is shown in Fig. 5. Experimental data for this reaction are generally known with better precision and also the calculation from the standalone version of GEF seems to reproduce the data very well, preferring the Budtz-Jørgensen data-set for $A < 100$. The DELFIN calculation shows a deviation with respect to data for masses $A > 150$.

4. Conclusions and outlook

The work presented here is still ongoing and only preliminary results are shown. It is however possible to make some observations.

The bump observed in the GEF-standalone $\bar{\nu}$(A) of ^{235}U (Fig. 2), ^{239}Pu (Fig. 4) and ^{252}Cf (Fig. 5) around mass $A = 140$ is not found in experimental data. It is also not reproduced when the same excitation energy and spin

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[1] In the case of the FREYA code, thermal fission is calculated for 0.5 MeV neutrons.

Table 1. Comparison of the evaluated average prompt $\bar{\nu}^{\bar{\nu}_{\mathrm{LF}}}_{\bar{\nu}_{\mathrm{HF}}}$ for the different reactions under study with that obtained using DELFIN with inputs from GEF, FREYA and PbP.

Reaction	$\bar{\nu}^{\bar{\nu}_{\mathrm{LF}}}_{\bar{\nu}_{\mathrm{HF}}}$ ENDF	$\bar{\nu}^{\bar{\nu}_{\mathrm{LF}}}_{\bar{\nu}_{\mathrm{HF}}}$ DELFIN		
	B-VII.1	GEF	FREYA	PbP
^{235}U(n,f)	$2.42\,^{1.39}_{1.05}$	$2.51\,^{1.36}_{1.14}$	$2.40\,^{1.12}_{1.28}$	$2.72\,^{1.61}_{1.11}$
^{239}Pu(n,f)	2.87	$2.90\,^{1.56}_{1.34}$	$3.01\,^{1.46}_{1.55}$	–
^{252}Cf(SF)	$3.76\,^{2.06}_{1.71}$	$3.92\,^{2.06}_{1.86}$	–	–

distributions are processed in DELFIN. This hints that this is a peculiarity of the de-excitation process built into GEF rather than a consequence of the E* partition at scission.

This is not the case, e.g., for the double-humped structure around the low-mass peak of ^{235}U and ^{239}Pu, that appears to be a direct consequence of the E* distributions. The shape is present in both FREYA and GEF, although the position of the humps and the minima differs between the two models (minima around mass 110/115 in Fig. 3 and mass 110/118 in Fig. 4 for FREYA/GEF, respectively). Yet, it does not seem to be replicated in experimental data, however uncertain these might be in proximity of the symmetric fission mass range due to the low yield.

From the $\bar{\nu}(A)$, assuming an initial mass yield distribution, it is also possible to extract the total $\bar{\nu}$ calculated in DELFIN. $\bar{\nu}$ is a value generally well known experimentally, especially for the systems we studied in this work. Along with it, some additional information can be inferred by the $\bar{\nu}_{\mathrm{LF/HF}}$, i.e. the average number of neutrons emitted by the light/heavy FF.

The results are shown in Table 1, where we can see how the majority of the analyzed codes tends to reproduce rather well the total $\bar{\nu}$. It is interesting to notice that in the calculations performed with FREYA E* as input, $\bar{\nu}_{\mathrm{HF}}$ is consistently larger than $\bar{\nu}_{\mathrm{LF}}$, unlike all the other codes and experimental data.

The results of the PbP model for ^{235}U(n$_{\mathrm{th}}$,f) (Fig. 3 and Table 1) show a striking difference with respect to data and the other models in the height of the sawtooth, especially for the light FF and total $\bar{\nu}$. This can most likely be explained by the fact that the E*(A) at full acceleration includes also a fraction of rotation energy that should not be available for neutron emission. Since this model does not include a calculation of E$_{\mathrm{rot}}$ we were not able to subtract this contribution [14].

We are now testing DELFIN with more models and reactions, studying other observables in addition to $\bar{\nu}(A)$. We are also developing a methodology based on the one developed for DELFIN to help in the identification of initial FF spins from isomeric yield ratios measurements [15].

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