# Model-based Generation of Neutron Induced Fission Yields up to 20 MeV by the GEF Code

**K. Kern*, M. Becker, C. Broeders, R. Stieglitz**

*Corresponding author: Kilian.Kern@kit.edu

INSTITUTE FOR NEUTRON PHYSICS AND REACTOR TECHNOLOGY (INR)

# Outline

# Outline

Introduction

Modelling of pre-fission processes

Modelling of fission product yields

Results

Conclusions

# Introduction

## Motivation

- Evaluated fission product distributions (JEFF 3.1) do not show a pronounced proton-even-odd effect
- Fission product distributions are given for maximum 3 energy intervals:

| | | |
|---|---|---|
| thermal | – | 400 keV |
| 400 keV | – | 14 MeV |
| 14 MeV | – | ? |

- Investigation of spectral effects of energy-dependent fission product yields in coupled criticality/depletion calculations (providing distributions in multi-energy-group representation)
- Model-based assessment of data uncertainties and covariances, of which the latter are not yet available in existing evaluated fission yields data libraries.

# Outline

Introduction

Modelling of pre-fission processes

Modelling of fission product yields

Results

Conclusions

# Modelling of pre-fission processes

## Applied nuclear reaction models

Karlsruhe Institute of Technology

A model description is needed not only for the fission process, but also for the formation of the excited fissioning nucleus. The TALYS-1.4 code has been applied for this purpose. It should be noted that:

- For a given target and incident neutron energy, TALYS calculates the probability for the fissioning nucleus to have proton and mass numbers $Z$ and $A$, excitation energy $E^*$ and spin/parity $J^\pi$.
- At incident neutron energies lower than the fission barrier of the target, the fission process is unlikely to be preceded by any nucleon emission (first-chance fission).
- At higher energies there is significant emission of nucleons, above all neutrons, before the nucleus undergoes fission (multi-chance fission).
- In any case, the excited nucleus may emit gamma quanta before it undergoes fission.

Below the (n,nf) second-chance fission threshold, fission is dominated by the direct (n,f) process, whereas in $^{235}$U(n,F) there is also a (n,$\gamma$f) contribution of roughly 10%. Sensitivities of modelled fission yields related to TALYS parameters thus show up mainly above the (n,nf) threshold.



INR

# Modelling of pre-fission processes

## Applied nuclear reaction models

Karlsruhe Institute of Technology

Summary of the essential models applied in the work with TALYS-1.4:

- Initial formation of the excited nucleus is described by optical model calculation with deformed potential from Soukhovitskiy using Coupled Channels partial wave expansion (CC) and Distorted Wave Born Approximation (DWBA), from which transmission coefficients and scattering/absorption cross-sections are obtained.
- For pre-equilibrium processes, i. e. decay reactions before the nucleus reaches statistical equilibrium, the exciton model and phenomenological descriptions are applied.
- Decay of an excited (equilibrated) compound nucleus is described by the Hauser-Feshbach formalism, which is very important for this work.

In this work, fission has been treated within the Hauser-Feshbach formalism and considered as a single-mode process by TALYS-1.4, which is the state-of-the-art method of fission cross-section modelling. Fission transmission coefficients have been calculated based on the Hill-Wheeler formula (here shown for a single-humped barrier):

$$P_F(E^* - \varepsilon) = \frac{1}{1 + \exp\left(-\frac{2\pi(E^* - E_F)}{\hbar\omega_F}\right)}$$

$$T_F(E^*, J^\pi) = \sum_i P_F(E^* - \varepsilon_i) + \int_{\varepsilon_c}^{E^*} d\varepsilon\, \rho_F(\varepsilon, J^\pi) \cdot P_F(E^* - \varepsilon)$$



INR

# Modelling of pre-fission processes

## Fission reactions

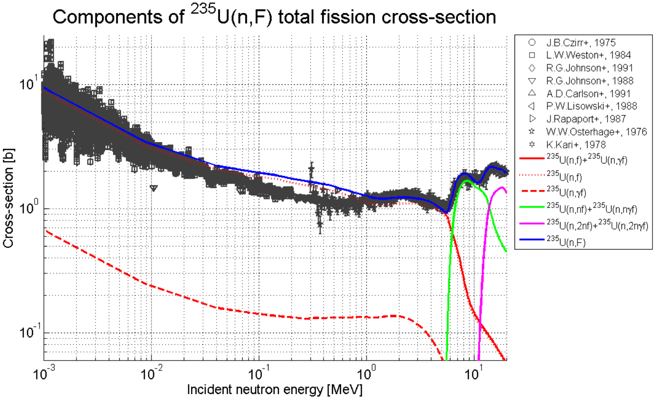



Figure 1: Below 5 MeV only first chance fission (solid red line), binary (n,f) reactions (dotted red line) dominating, pre-fission gamma emission (dashed red line) factor 10 smaller. Second (green line) and third chance fission (pink line) are very important above their respective thresholds.

# Outline

# Modelling of fission product yields

## Applied nuclear reaction model

Karlsruhe Institute of Technology

In the frame of physical constraints and arguments, the GEF model uses empirical descriptions for a number of effects. This way, it provides a realistic reproduction not only of the yields of fission fragments, but also of their initial excitation energy and spin as well as their deexcitation. Several important principles are applied in the modelling of fission fragment formation:

- **Inertia of degrees of freedom:** Known from theoretical calculations to be high for fragment mass numbers, but low for $N/Z$ ratio. Hence, mass numbers assumed to be fixed at outer fission barrier during fission process, but $N/Z$ later at scission point.
- **Separability principle:** Nascent fragments determine microscopic potential (shell and pairing effects) of fissioning nucleus, which interplays with the macroscopic potential. Corroborated by two-center shell model calculations of Mosel and Schmitt [].
- **Energy sorting mechanism:** Nascent fragments assumed to have not only their own microscopic potential, but also their own intrinsic temperature. This affects the division of intrinsic excitation energy among the fragments and gives an explanation of experimental observations.
- **Phenomenological description** for the central values and variances of fragment yield distribution with respect to fragment mass number and $N/Z$ ratio.

# Modelling of fission product yields

## Applied nuclear reaction model

The formation of fission fragments and their deexcitation is treated in the following way:

- **Multi-mode fission** model: Weights of fission modes are determined from ratios of Hill-Wheeler transmission coefficients for the respective outer fission barrier. Result depends on $Z$, $A$ and $E^*$ of fissioning nucleus.
- Fission fragment formation is calculated for each fission mode;
  $Z$, $A$, $E^*$ and mean $J$ of fragments are determined.
- GEF uses the **Weisskopf-Ewing formalism** for fragment deexcitation, i. e. the impact of fragment spins is neglected at first. Spin $J$ of fragments only affects population of isomeric states in GEF model.
- Fragments are assumed to deexcite by **neutron and E1 gamma emissions** until $E^*$ reaches the **yrast line**.
- Subsequent gamma emissions down to the ground or isomeric state are assumed to be **E2 transitions**.

# Modelling of fission product yields

## Calculation of fission yields and covariance matrix

GEF fission yields have been generated in a Monte Carlo calculation for each bin of the fission contribution obtained from TALYS, setting the statistics of each bin in $Z$, $A$, $E^*$ and $J$ of the compound nucleus proportional to the calculated probability. The covariance matrix of FY has in turn been determined in a second run divided into $N = 224$ calculation steps with perturbed model parameters:

$$V_{ij} = \frac{1}{N} \cdot \sum_{k=1}^{N} \left(y_{i,k} - \overline{y}_i\right) \cdot \left(y_{j,k} - \overline{y}_j\right)$$

- Total number of fission events in each calculation: $5 \cdot 10^7$, thus the statistical uncertainties of most yields are negligible compared to impacts of model parameter uncertainties.
- GEF propagates estimated, uncorrelated parameter uncertainties.
- Parent independent yields and their uncertainties have been obtained from GEF.
- In calculation of parent cumulative yields and their uncertainties, covariances of independent yields and decay data have still been neglected.

# Outline

Introduction

Modelling of pre-fission processes

Modelling of fission product yields

Results

Conclusions

# Results

## Parent independent yields - thermal neutrons

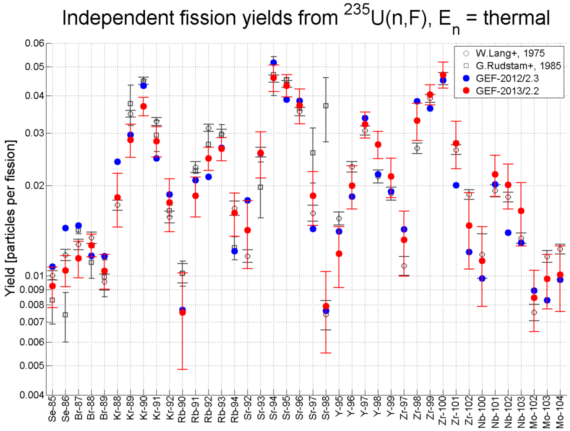



Figure 2: Independent fission product yields from $^{235}$U(n,F) induced by thermal neutrons. Results from GEF-2012/2.3 (still without uncertainty assessment) and GEF-2013/2.2 compared to EXFOR

# Results

## Parent cumulative yields - thermal neutrons

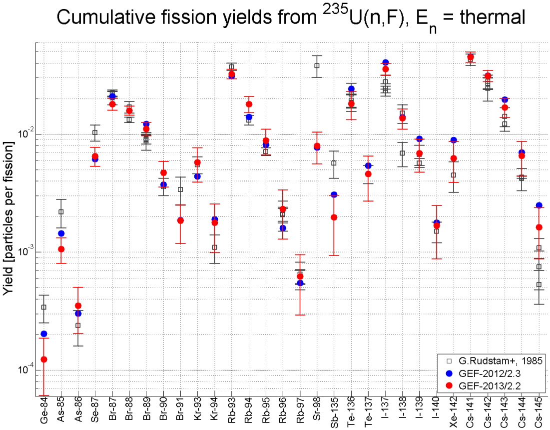



Figure 3: Cumulative fission product yields from $^{235}$U(n,F) induced by thermal neutrons, calculated from independent yields using ENDF/B-VII.1 decay data library. GEF results compared to EXFOR

# Results

## Parent cumulative yields - high energetic neutrons

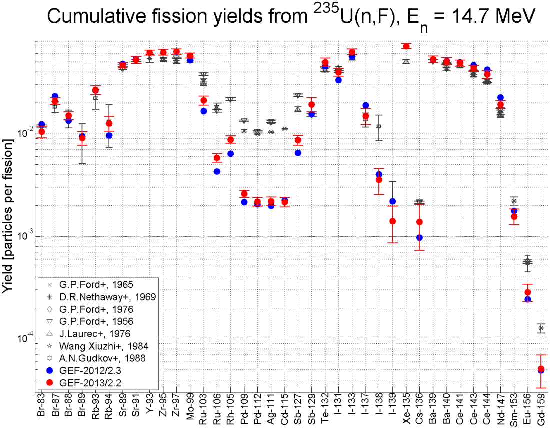



Figure 4: Cumulative fission product yields from $^{235}U(n,F)$ induced by 14.7 MeV neutrons. Significant underestimation of FPY from the superlong mode around $A = 115$.

# Results

## Measuring the quality of model results

To measure the quality of the calculated fission product yields and their uncertainties, two test quantities $H$ and $\widetilde{H}$ have been calculated, corresponding to a reduced-$\chi^2$ test:

$$H = \sqrt{\frac{1}{N} \cdot \sum_{i=1}^{N} \frac{\left(y_i^{\text{exp}} - y_i^{\text{calc}}\right)^2}{\sigma^2_{y_i^{\text{exp}}}}} \qquad \widetilde{H} = \sqrt{\frac{1}{N} \cdot \sum_{i=1}^{N} \frac{\left(y_i^{\text{exp}} - y_i^{\text{calc}}\right)^2}{\sigma^2_{y_i^{\text{exp}}} + \sigma^2_{y_i^{\text{calc}}}}}$$

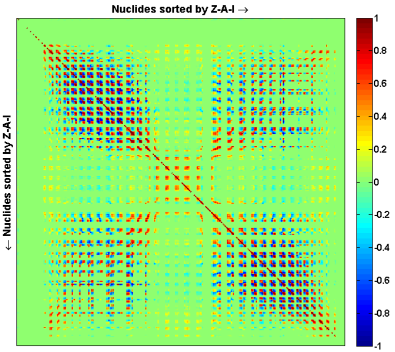
The following values were obtained:

Table 1: Values of $N$, $H$ and $\widetilde{H}$ for Figures 2-4.

| Figure | $N$ | $H$, $\widetilde{H}$ 1$\sigma$ confidence interval | $H$ GEF-2012/2.3 | $H$ GEF-2013/2.2 | $\widetilde{H}$ GEF-2013/2.2 |
|---|---|---|---|---|---|
| 2 | 60 | 0.913 - 1.097 | 4.52 | 3.50 | 1.12 |
| 3 | 51 | 0.906 - 1.106 | 5.10 | 3.98 | 1.26 |
| 4 | 69 | 0.919 - 1.090 | 21.97 | 20.83 | 11.20 |

# Results

## Fission yields correlation matrix



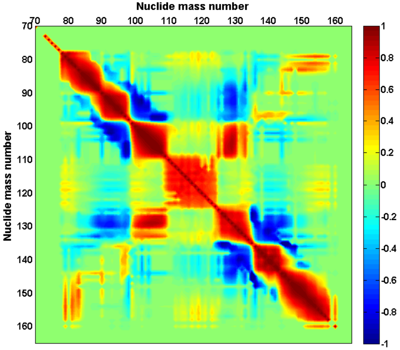




Figure 5: Plot of correlation matrix of fission product yields for 235 U(n,F) induced by thermal neutrons. Yields given as a function of proton number, mass number and isomer (left) or only as a function of mass number (right). Visible anticorrelations originate from proton even-odd effect and competition between fission channels.

# Outline

Introduction

Modelling of pre-fission processes

Modelling of fission product yields

Results

Conclusions

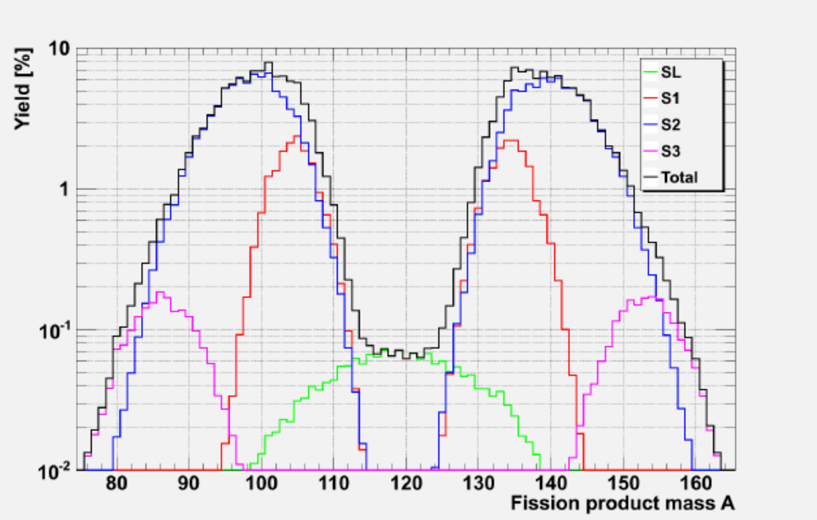
# Conclusions

Karlsruhe Institute of Technology

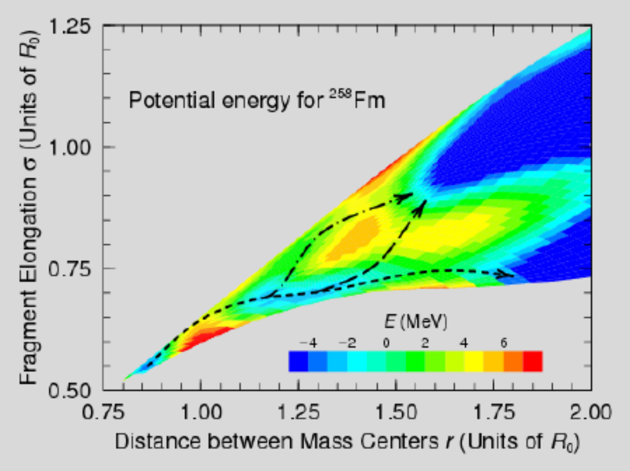
- General improvement of FPY modelling with switch from GEF-2012/2.3 to GEF-2013/2.2.
- Realistic estimation of FPY uncertainties for parent independent FPY from $^{235}$U(n,F) induced by thermal neutrons.
- Underestimation of FPY uncertainties for parent cumulative FPY from $^{235}$U(n,F) induced by thermal neutrons, which might be resolved by consideration of independent FPY and decay data covariances.
- Deviation in 14.7 MeV cumulative FPY in Figure 4 should be resolved by adjustment of fission barrier parameters for superlong mode in GEF. The weight of this mode is a very sensitive quantity.
- Still room for improvement of FPY modelling, as also shown by the values of *H* in Table 1.
- Inconsistency between models of TALYS-1.4 and GEF: Single-mode fission vs. multi-mode fission; multi-mode fission should already be considered in calculation of fission contribution as it is possible e. g. with the EMPIRE-3.2 code; parameters of coupled codes should be identical. However, this would significantly increase the number of model parameters to be fitted for fission cross-section calculations.

# Backup

# Multichannel fission of Pu-241



# Potential energy of Fm-258



# Proton Even-Odd effect