# Implementation of a Monte-Carlo-type fit procedure in GEF

## Implications for the description of anti-neutrino production in fission

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TM on Nuclear Data Needs for Antineutrino Spectra Applications,
IAEA, Vienna, 16-20 Jan 2023

# Introduction

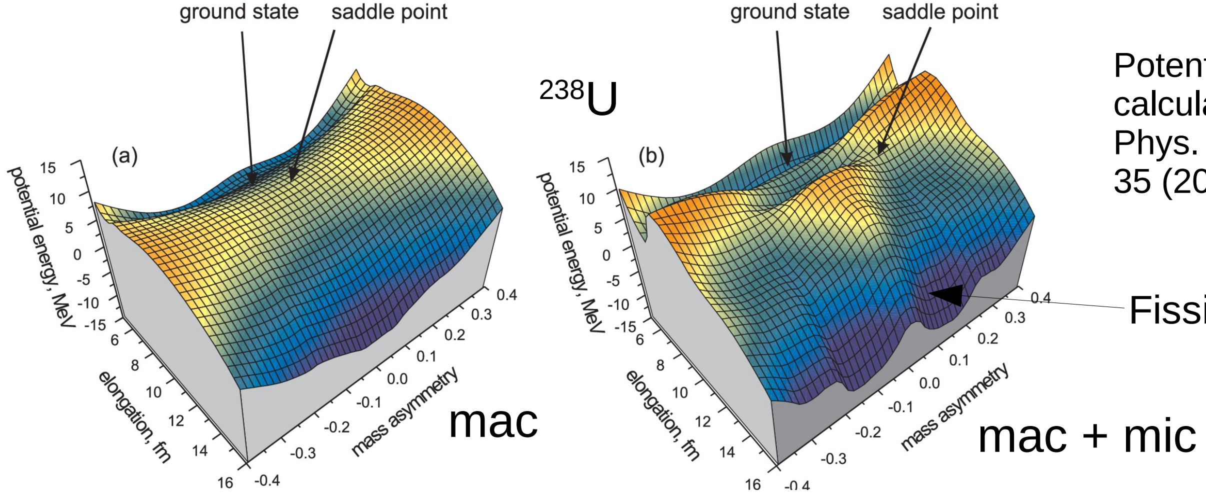
- The summing method is now a standard for anti-neutrino calculations.
- It requires fission-fragment yield (FY) data on input.
- Possible sources of FY data are
  - Measured FY (incomplete, inconsistent)
  - Traditional evaluations (for few systems)
  - Systematics
  - **Semi-empirical GEF model (physics + adjustable parameters, global description for all systems, applicable to systems without measured data.)**
  - Microscopic physics-based models (insufficient accuracy, difficult to adjust to accurately measured data)

*Less physics*

*More physics*

# GEF

**The evolution of the system on the potential-energy surface is a basic concept of GEF.**




Potential-energy surface calculated by Karpov et al., Phys. G: Nucl. Part. Phys. 35 (2008) 035104

Quantum-mechanical structure forms fission valleys.

GEF needs to handle:

- Division of the flux between the different fission valleys
- Fluctuations inside the fission valleys in mass-asymmetry, N/Z, shape
- Division of excitation energy between the nascent fragments
- Emission of prompt neutrons and gammas
- Radioactive decay (beta decay, antineutrinos, delayed neutrons, cumulative yields)

**GEF covers the whole fission process.**
**Values of GEF parameters determined by a fit to all kind of fission data.**

# Considerations about finding the optimum parameters of GEF

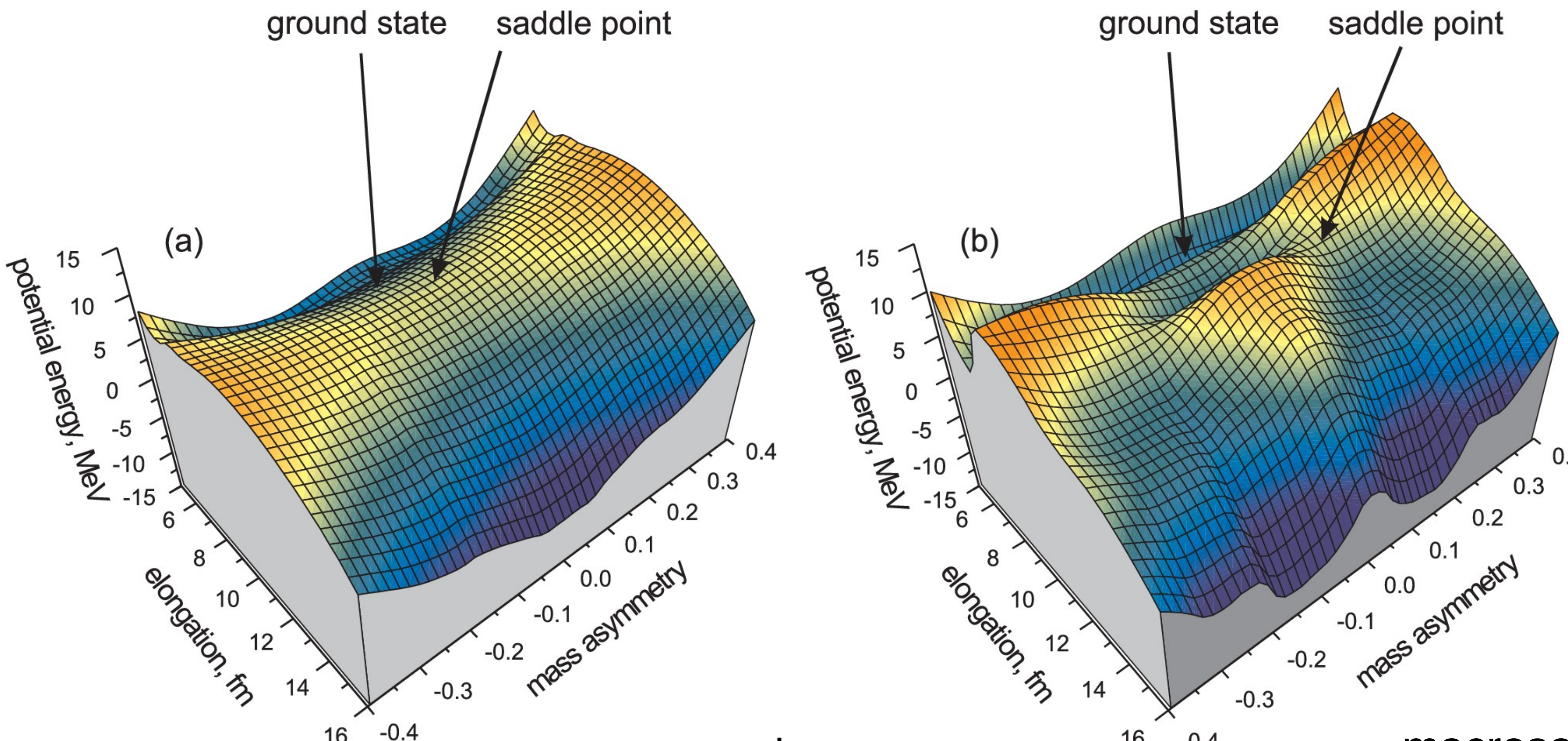
- Availability of basic empirical data is limited. Data quality is critical, selection is required.
- Difficulty to weight the data of different nature.
- Difficulty to consider correlations in the data.
- GEF calculations need high statistics to suppress statistical fluctuations that disturb the influence of the parameters.
- Analytical fitting algorithms cannot be used due to the statistical fluctuations of the GEF results.

# Methods for parameter fitting

- **Possibilities and limitations of the eye fit** (used up to now)
  - (+) Intuitive relations between GEF parameters and observables
  - (-) Subjective method
  - (-) Cumbersome
  - (-) Too complex for finding the objective „best“ parameters
- **Possibilities and limitations of the Monte-Carlo fit** (new)
  - (+) Objective method
  - (+) Parameter search enhanced by computing power
  - (-) Decoupled from intuitive understanding
- **Combination** (benefit from both methods)
  - Deduce the physics of GEF from an eye fit
  - Determine the optimum parameter values of GEF by Monte-Carlo fit

# Potential energy

Calculation by Karpov et al., Phys. G: Nucl. Part. Phys. 35 (2008) 035104



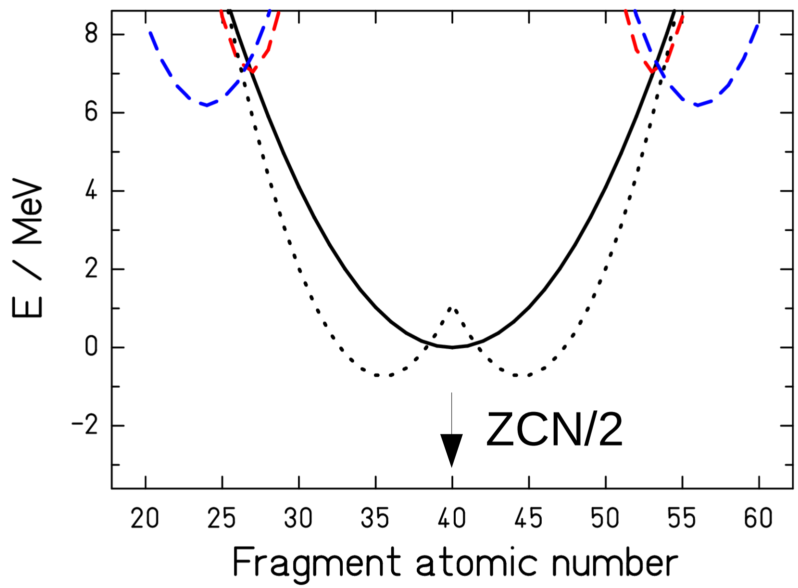

macroscopic

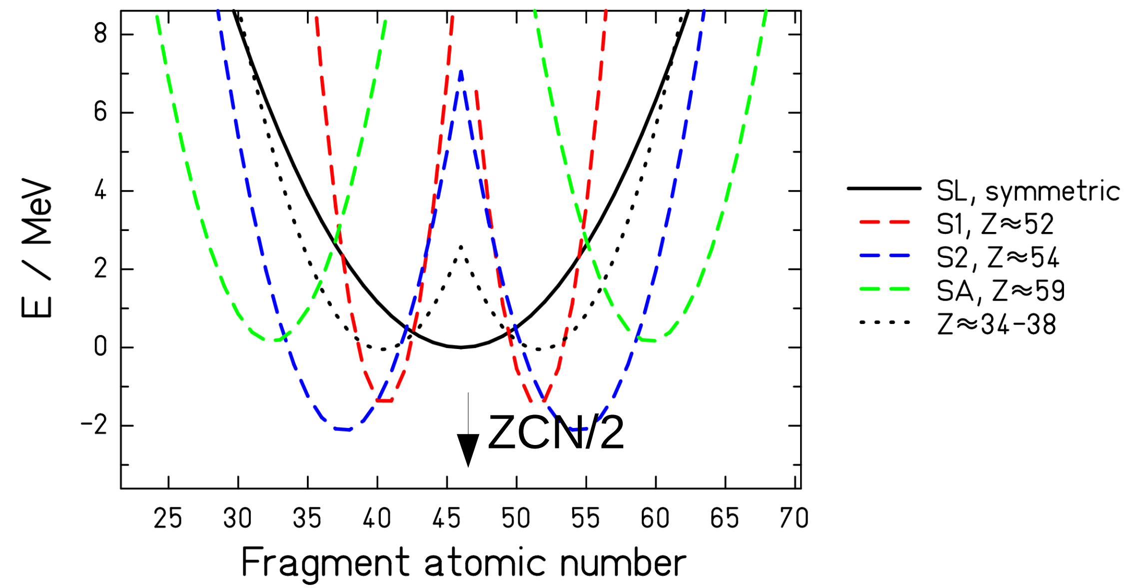
macrosopic + microscopic

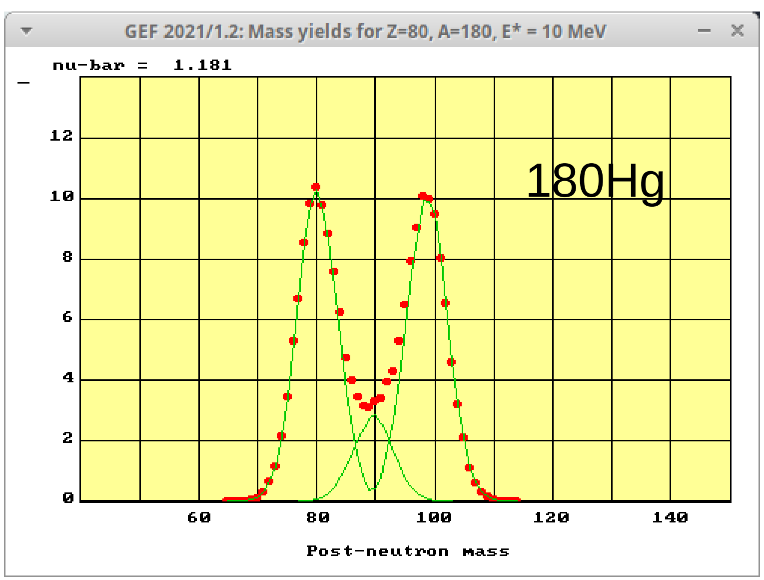
**Quantum-mechanical structure forms fission valleys.**

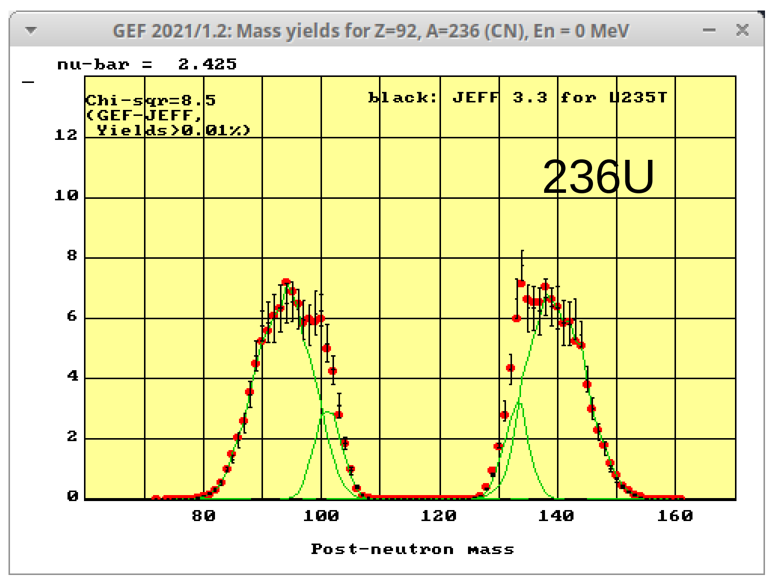
GEF:
Simplified model of the potential-energy landscape:
position, depth and width of the fission valleys

# GEF uses the same 4 proton shells for all systems



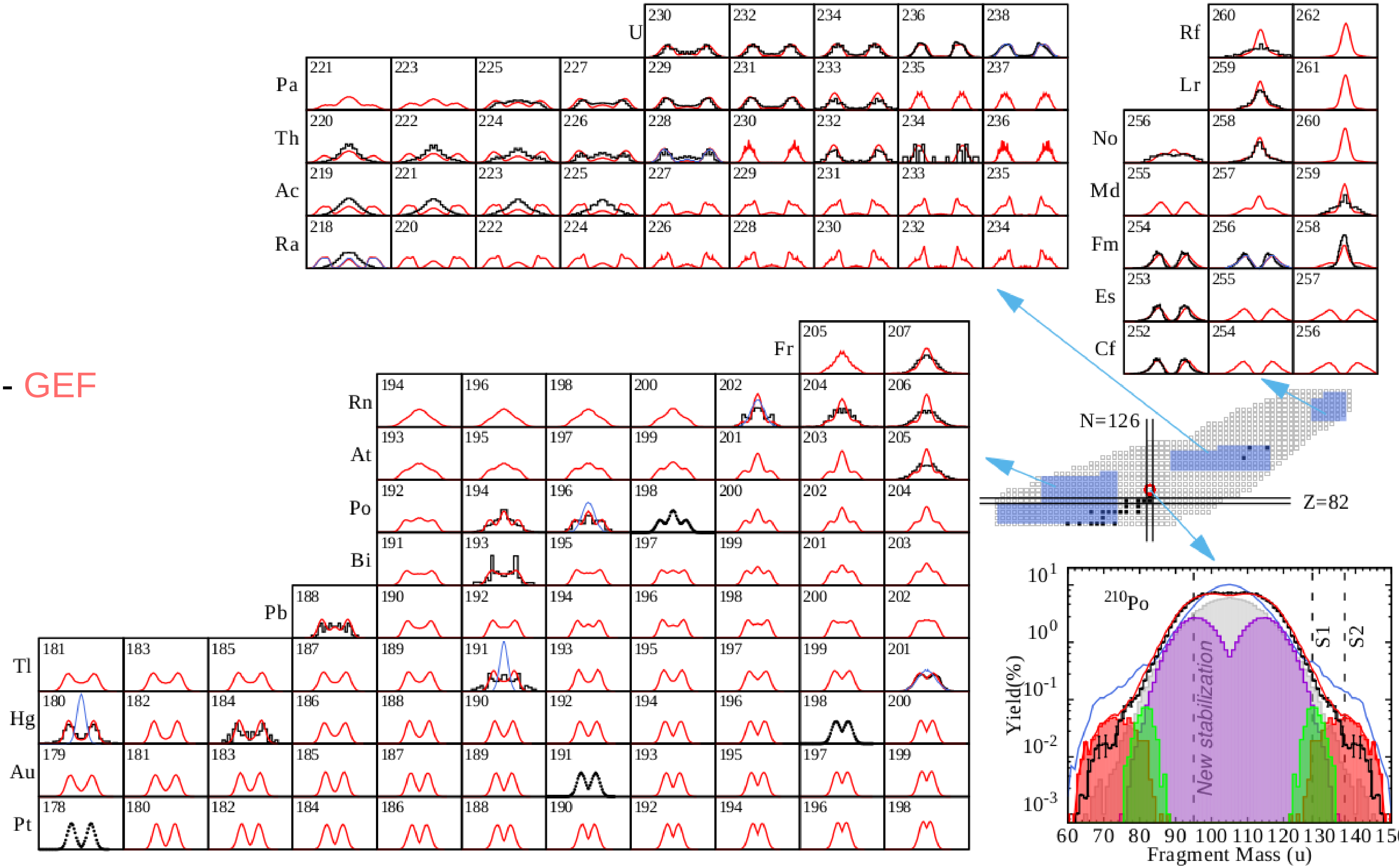




→ Simultaneous description of all fissioning systems
with a unique parameter set! (Only the mac potential varies.)

# GEF with parameters from eye fit: Overall benchmark

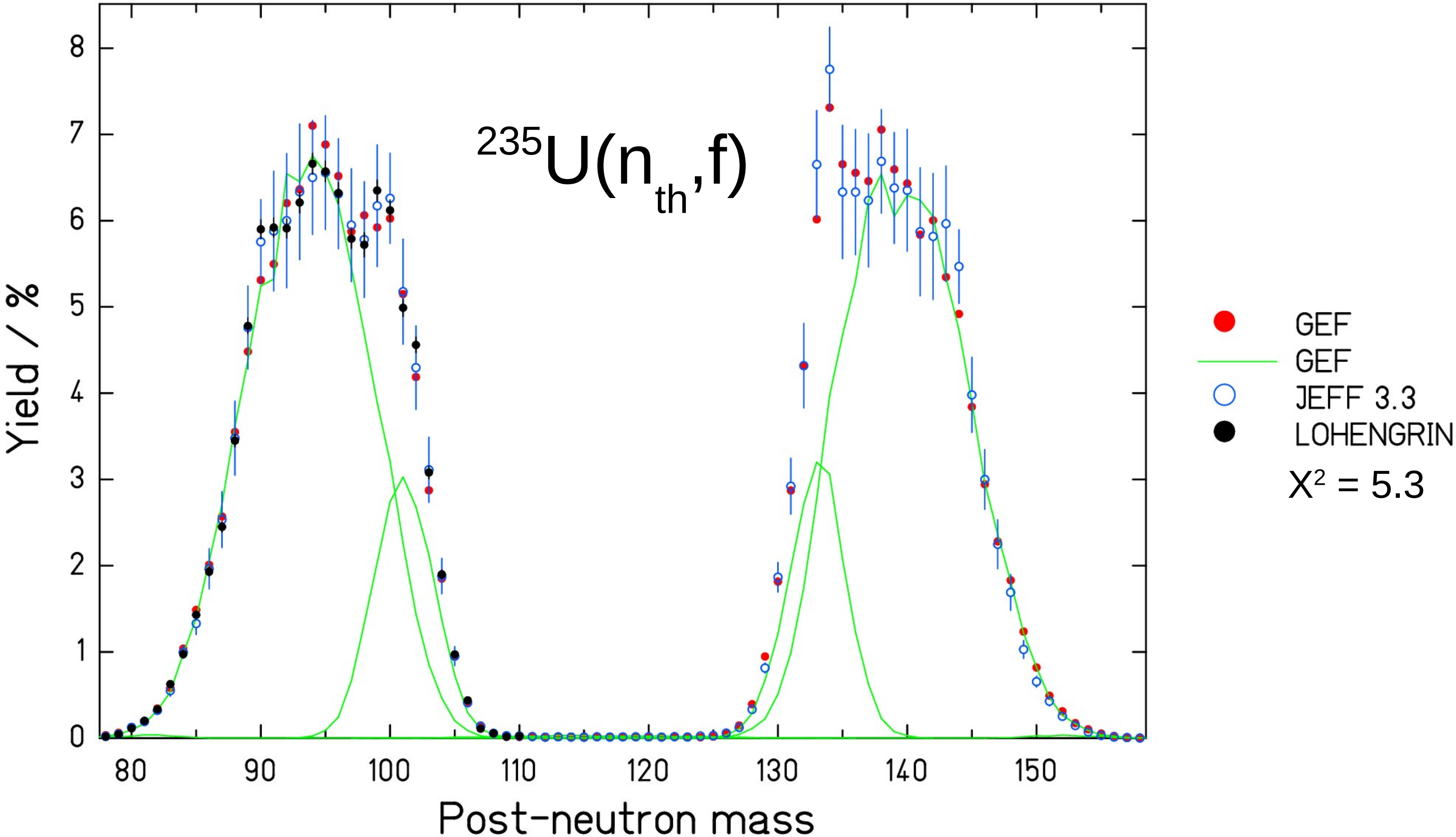
exp - GEF




K. Mahata, et al., Phys. Lett. B 825 (2022) 136859

# Global eye fit

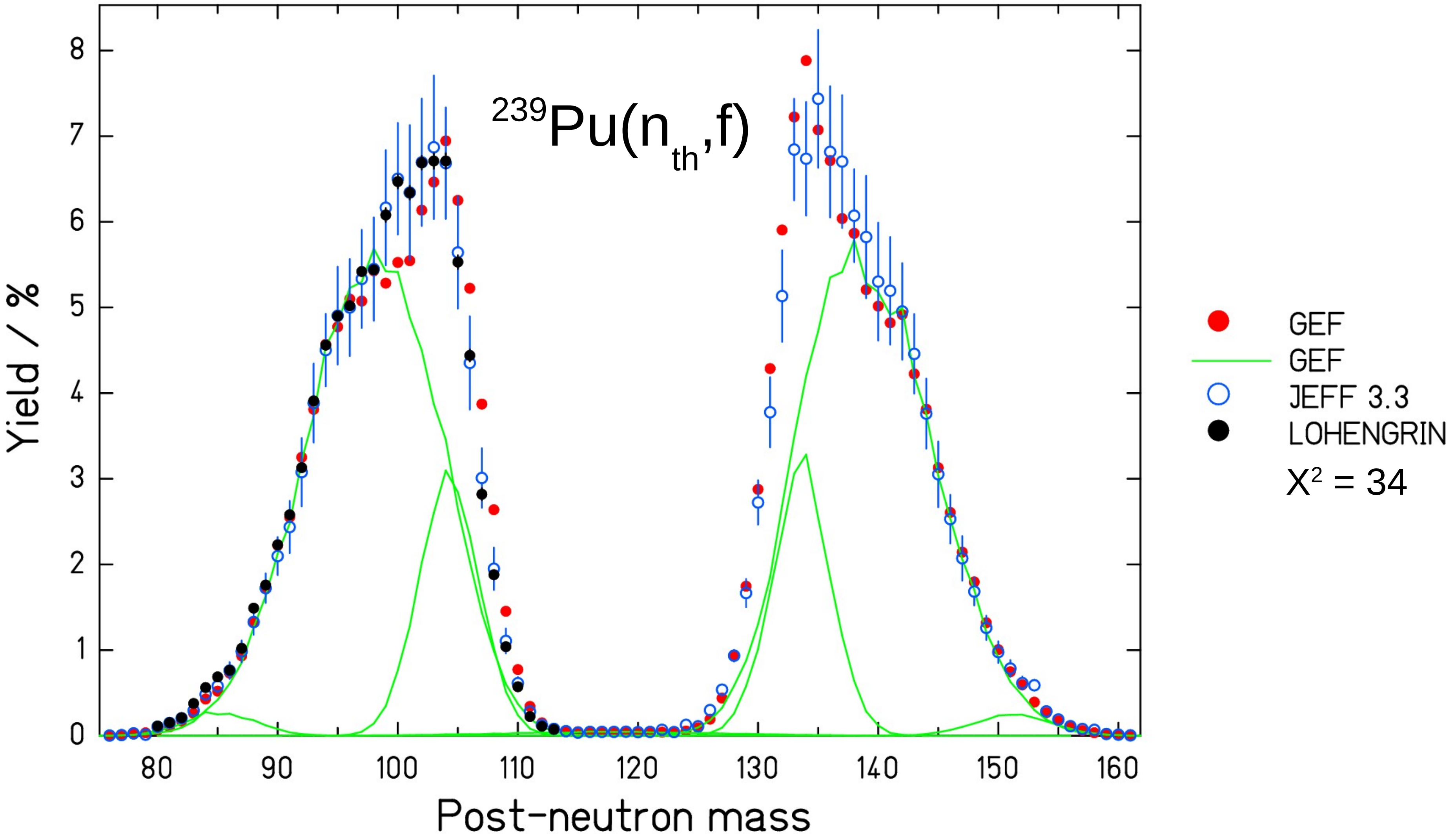
Strong influence from $^{235}U(n_{th},f)$ and $^{252}Cf(sf)$ !




Most important source of anti-neutrinos in reactors.
Good reproduction, some deviations near the peaks.

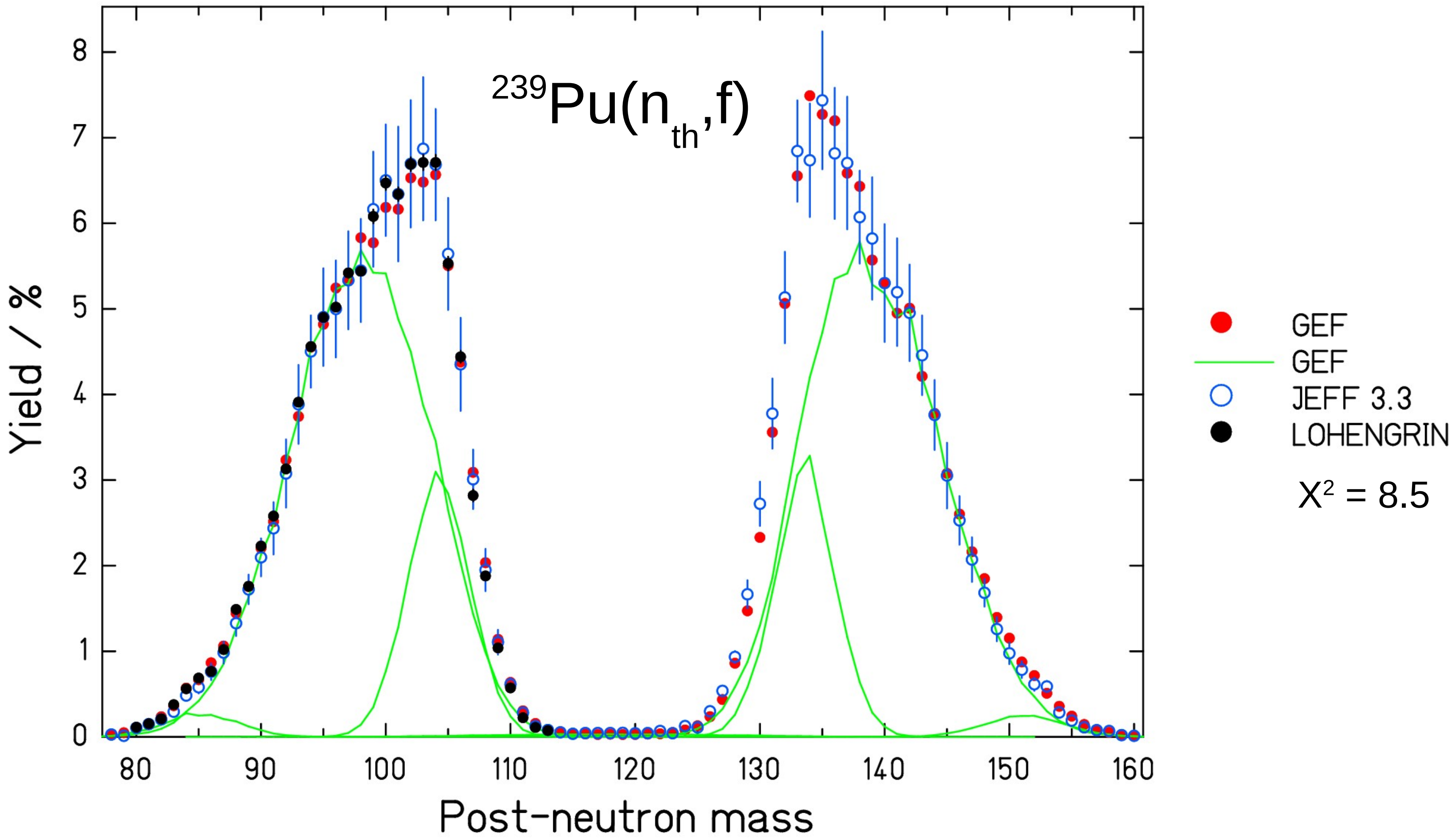
# Global eye fit

## Strong influence from $^{235}U(n_{th},f)$ and $^{252}Cf(sf)$ !



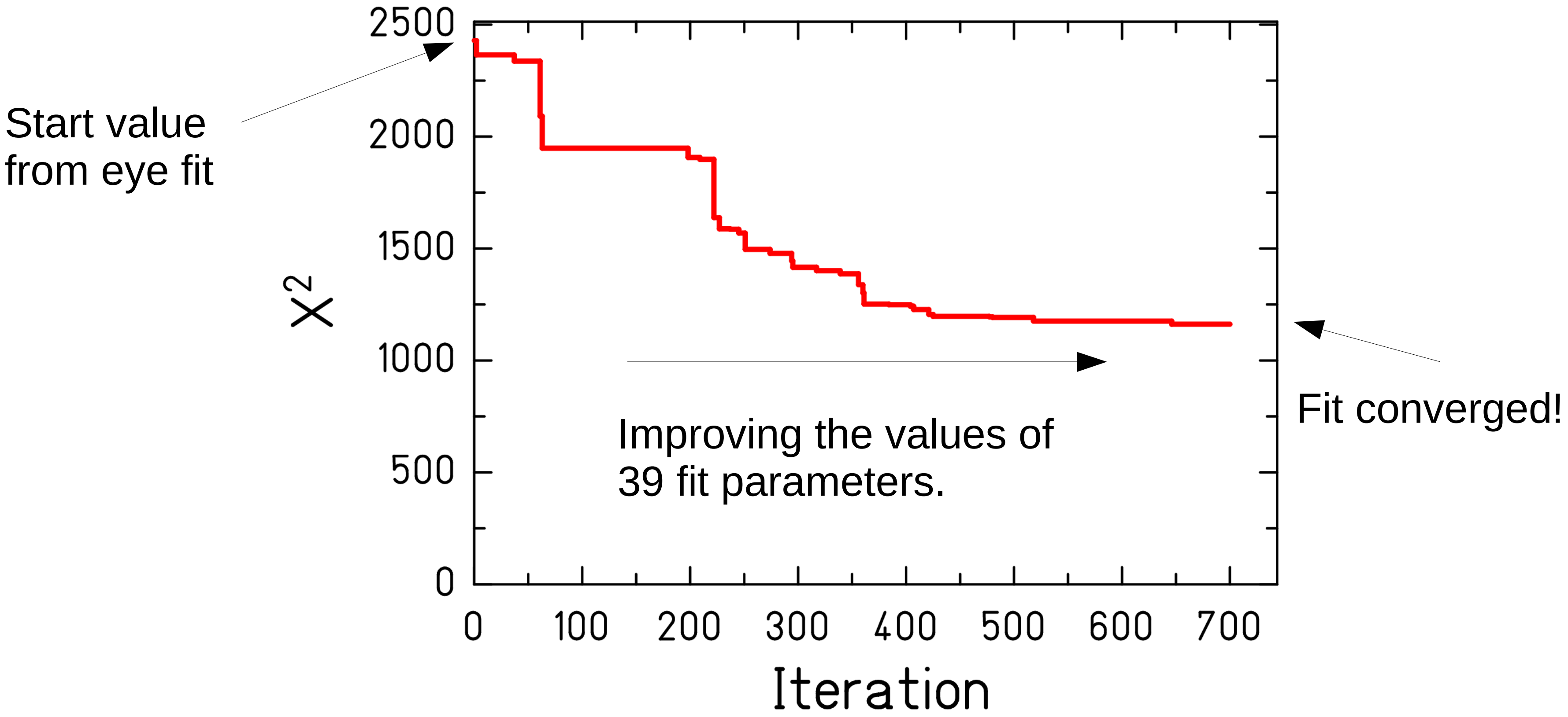

Another important source of anti-neutrinos in reactors.
Fair reproduction, larger deviations.

# GEF parameters locally adjusted to $^{239}Pu(n_{th},f)$




Local adjustment gives better reproduction for specific systems, but not satisfactory in view of the predictive power of GEF.

# Implementation of a Monte-Carlo fit procedure in GEF




Starting from the result of the eye fit, the Monte-Carlo fit reduces the Chi-square further by a considerable amount.

# Success of the
# Monte-Carlo fit procedure

Chi-square values
(deviations from Lohengrin data)
for the two systems:

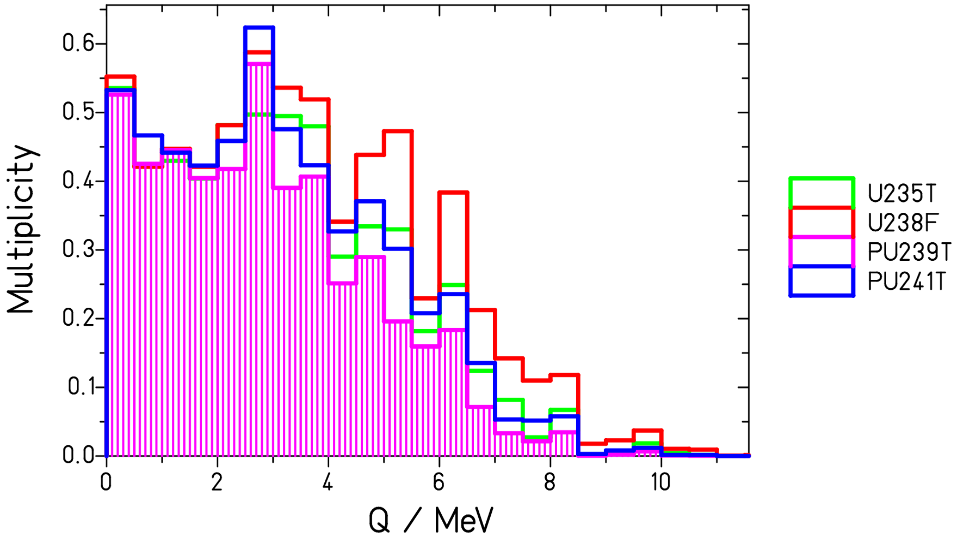
| | Global eye fit to all systems | Local eye fit specific to 239Pu(nth,f) | Monte-Carlo fit to all systems |
|---|---|---|---|
| 235U(nth,f) | 5.3 | 20 | 5.4 |
| 239Pu(nth,f) | 34 | 8.5 | 13 |

Monte-Carlo fit yields a good description for 235U(nth,f) and 239Pu(nth,f) with the same parameter set.

# Status and outlook

- Eye fit provides already a rather good global description of fission yields.
- The newly implemented Monte-Carlo fit is better suited to find the objective „best“ parameter values.
- This should enhance the reliability and predictive power of GEF, also for anti-neutrino production.
- Benchmark of the new GEF version for anti-neutrino production requires collaboration with specialized group(s).

A sample of available GEF results:




Antineutrino multiplicities as a function of the Q value of the consecutive FF beta decays. (Previous GEF parameters of the eye fit used from Nucl. Data Sheets 173 (2021) 54.) Can be calculated for any fissioning system!

# Appendix:
# What about machine learning?

- Application of A.I. for calculating FY without constraints violates all kind of consistency requirements, for example:
  - 2 fragments per fission in the same mode,
  - conservation of mass, charge and energy.
- The need for introducing the necessary constraints is equivalent of using a physics model as a basis directly.
- Pure machine learning cannot make use of the powerful physics concepts exploited in GEF.
- Machine learning may be helpful for deducing remaining deficiencies in the physics of GEF by searching for residual systematic discrepancies.

# Backup

# Parameters (most important ones)

- **Position, depth and width of 4 shells (→ fission modes)**
- Charge polarization (→ N/Z displacement)
  (specific to the fission channel)
- ZPM of charge displacement (→ N/Z)
- Dissipation fraction (saddle to scission) (→ E*)
- Fraction of collective exc. (saddle to scission) (→ E*)
- Elongation of nascent fragments (f(Z)), specific to the fission channel (→ Deformation energy → E*)

## Data used for adjusting the parameter values

- Post-neutron fission yields (masses and isotopes)
- Isomeric ratios
- Total kinetic energies
- A-dependent prompt-neutron multiplicities
- Delayed-neutron yields
- Decay heat
- Anti-neutrino multiplicities and spectra *)
- and others

*) K.-H. Schmidt et al., Nucl. Data Sheets 173 (2021) 54