# Recent work on the GEF code

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# Summary

- The following slides taken from work by Karl-Heinz Schmidt, Beatriz Jurado and Charlotte Amouroux

- GEF - an approach to fission based on fundamental laws of physics and mathematics
- Assessment of GEF model
- Validation of GEF results
- Covariances from GEF/MATCH

See preprint and website for further details

# Existing fission models

- Empirical models:
  + Adjustment to data by simple fit.
  + Good preproduction of data.
  - Low predictive power.
- Stochastic models (solution of Langevin equations):
  + Predictive power by general adjustment to nuclear properties.
  + Aspects of statistical mechanics fully considered.
  - Adjustment to data complicated and indirect.
  - Classical model (missing features of quantum-mechanics).
  - Low precision due to uncertainties in model parameters.
  - Restricted by limited computing power.
- Self-consistent models (dynamical Hartree-Fock calculation):
  + Based on quantum-mechanics.
  - Adjustment to data complicated and indirect.
  - Low precision due to unknown nuclear force.
  - Aspects of statistical mechanics not sufficiently developed.
  - Restricted by limiting computing power.

# Concept of the GEF model

- **General approach using global theoretical models and considerations on the basis of universal laws of physics and mathematics.**
- Topological properties of a continuous function in multi-dimensional space. (→ Fission barriers.)
- Condensation of matter at low *T*. (→ Level densities.)
- Evolution of quantum-mechanical wave functions in systems with complex shape. (→ Fragment shells.)
- Memory effects in the dynamics of stochastic processes. (→ Dynamical freeze-out.)
- Influence of the Second Law of thermodynamics on the evolution of open systems. (→ Energy sorting.)

# Fission barriers

- Weak points of calculated fission barriers:
  Low precision in structural effects.
  Long-range trend (with *N/Z*) controversial.
- Topographical theorem:
  Structural effects dominated by ground state.
  Calculation can be replaced by precise information from measured masses.

GEF: RMS deviations [MeV] lower than RIPL 3.

| | exp | RIPL3 | GEF | Goriely | Möller |
|---|---|---|---|---|---|
| exp | | 0.43 | 0.20 | 0.37 | 1.1 |
| RIPL3 | 0.43 | | 0.46 | 0.46 | 1.0 |
| GEF | 0.20 | 0.46 | | 0.38 | 1.1 |
| Goriely | 0.37 | 0.46 | 0.38 | | 1.0 |
| Möller | 1.1 | 1.0 | 1.1 | 1.0 | |

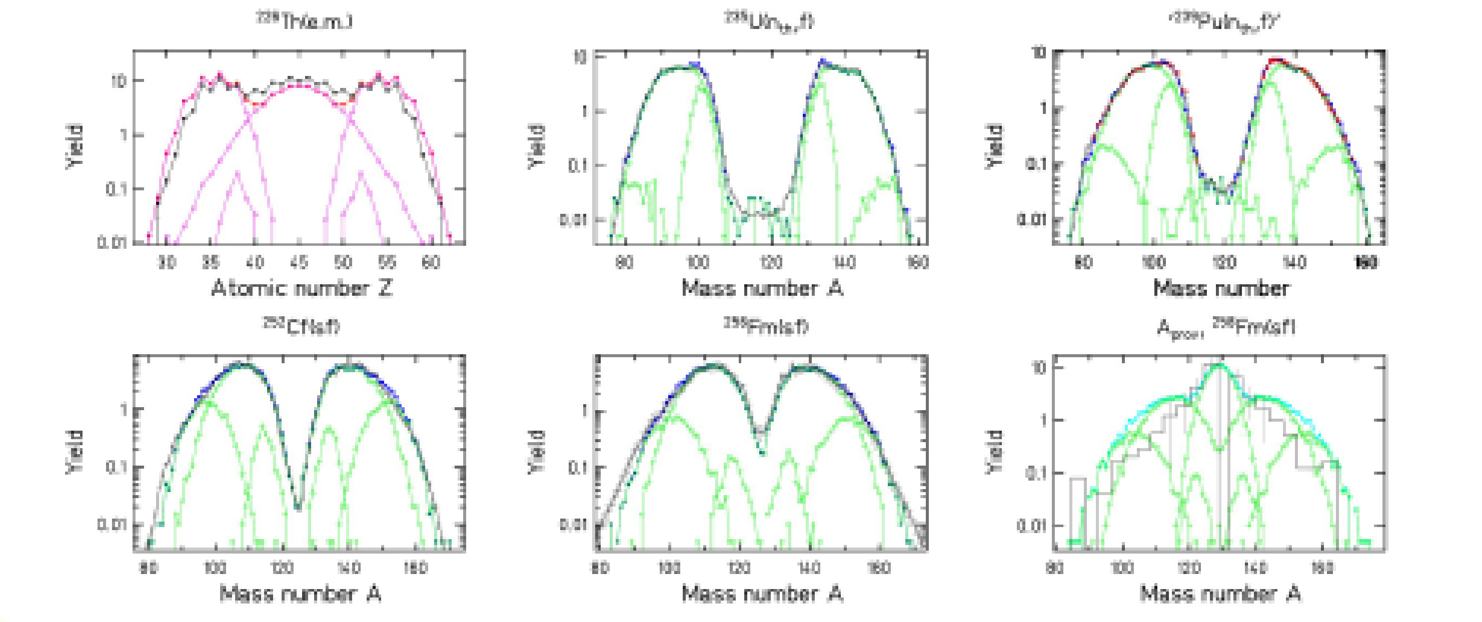
# Nuclear level density

- General property of matter:
  Gain of binding energy by freezing part of the degrees of freedom at low T.
  (gas → liquid, liquid → solid or fluid → superfluid)
- Application to nuclei:
  **High T**: Independent-particle regime.
  → Fermi-gas level density: $\rho \sim \exp(2\sqrt{(aE)})$
  **Low T**: Residual interactions (e.g. pairing) increase heat capacity.
  → Constant-temperature level density.: $\rho \sim \exp(E/T)$
- Most level-density formulae violate these basic rules.

Inconsistencies in the description of pairing effects in nuclear level densities, K.-H. Schmidt, B. Jurado, Phys. Rev. C 86 (2012) 044322

# Fission channels

- "Fission valleys" in the potential-energy surface are produced by fragment shells.
- Fragments shells depend on $Z_1, N_1, Z_2, N_2$ for all fissioning systems (hidden systematics behind complex features of mass distributions).




- Experimental evidence for the separability of compound-nucleus and fragment properties in fission, K.-H. Schmidt, A. Kelic, M. V. Ricciardi, Europh. Lett. 83 (2008) 32001

# Dynamics

- Dynamical effects are important.
- Empirical fragment shells include dynamical effects (early freeze-out).
- Dynamical memory time is specific:
  short for N/Z,
  longer for A.

# Energy sorting

- Distribution and transformation of energy is driven by entropy (statistical mechanics).
- Influence on mass-dependent prompt-neutron yields.
- Influence on even-odd effect in Z yields.

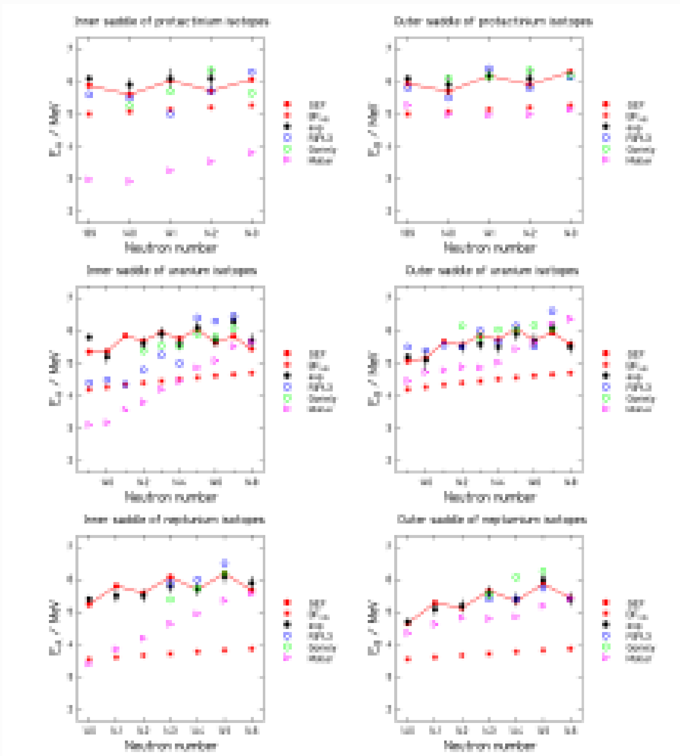

- Entropy-driven excitation-energy sorting in superfluid fission dynamics, K.-H. Schmidt, B. Jurado, Phys. Rev. Lett. 104 (2010) 212501
- Thermodynamics of nuclei in thermal contact, K.-H. Schmidt, B. Jurado, Phys. Rev. C 82 (2011) 014607
- Final excitation energy of fission fragments, K.-H. Schmidt, B. Jurado, Phys. Rev. C 83 (2011) 061601(R)
- New insight into superfluid nuclear dynamics from the even-odd effect in fission, K.-H. Schmidt, B. Jurado, arXiv:1007.0741v1 [nucl-th]

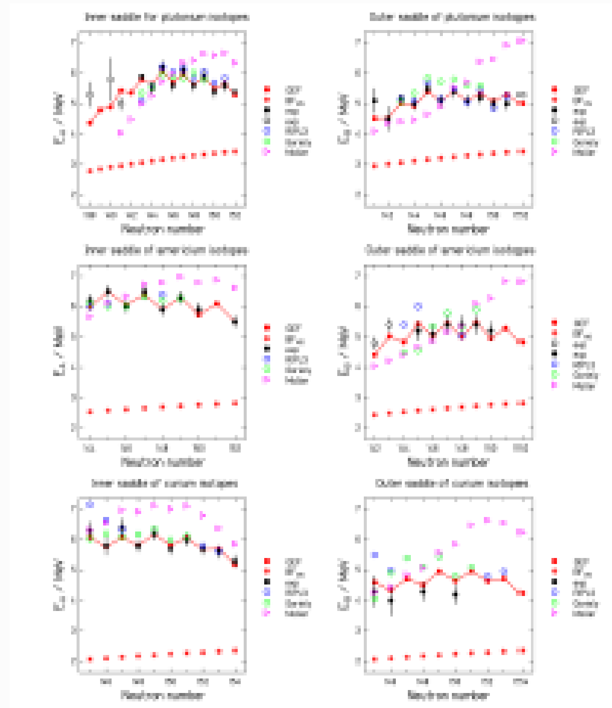
# Conclusion

- Universal laws of physics and mathematics establish a rigid theoretical framework.
- Quantitative calculations depend on the values of a limited number of parameters*), which are determined in a comprehensive fit to great part of the large body of various experimental data.
- The model allows predicting the behaviour of a specific system without any particular experimental information.
- Fast code → 5 seconds for $n_{th}$,f.
- Precision suited for nuclear technology.
- Useful tool for validation and evaluation.

Around 50 parameters for hundreds of systems + variation with E*.

# Fission barriers





GEF:
Based on the topographical theorem (Myers & Swiatecki).

| | exp | RIPL3 | GEF | Goriely | Möller |
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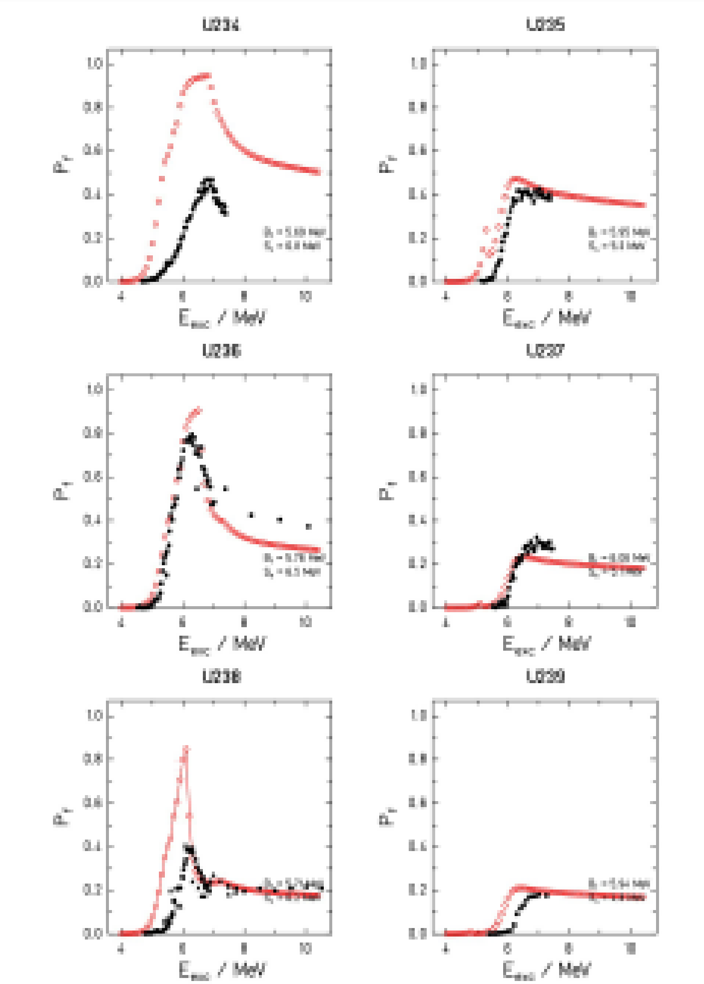
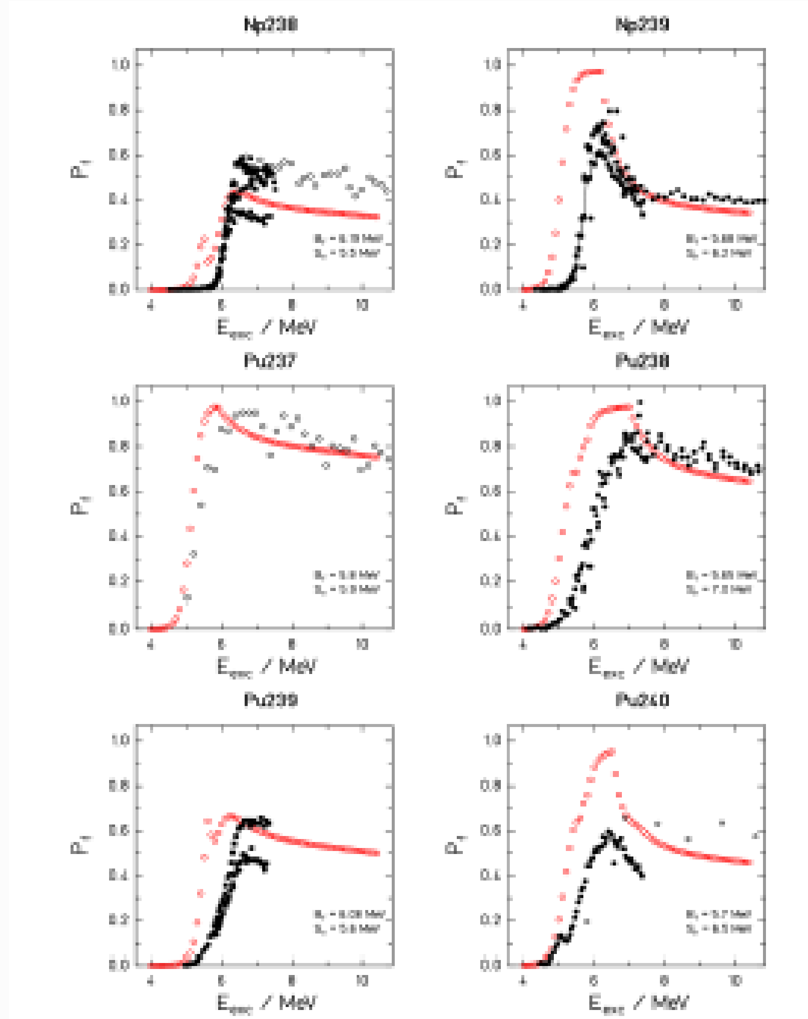
← RMS deviation [MeV]

GEF vs exp (0.2 MeV)
=
uncertainty of the experimental data!

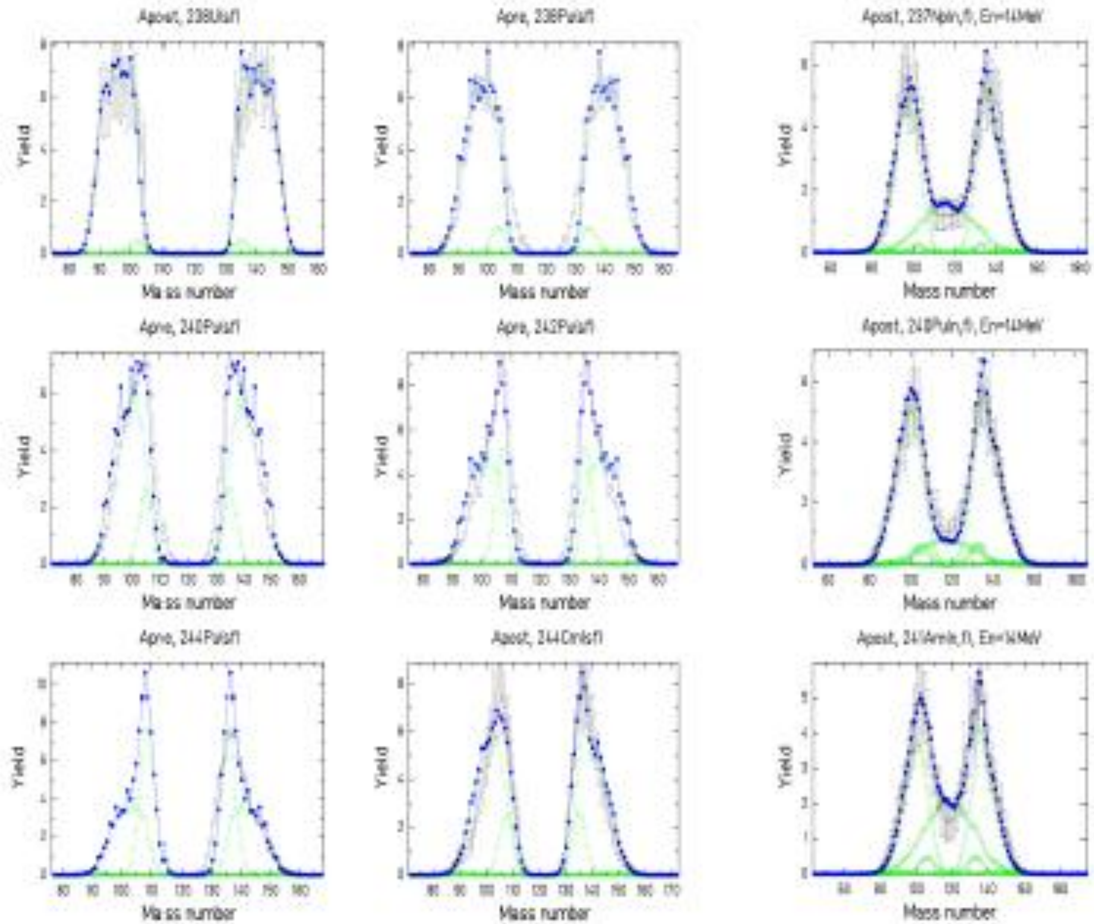
# Fission probabilities

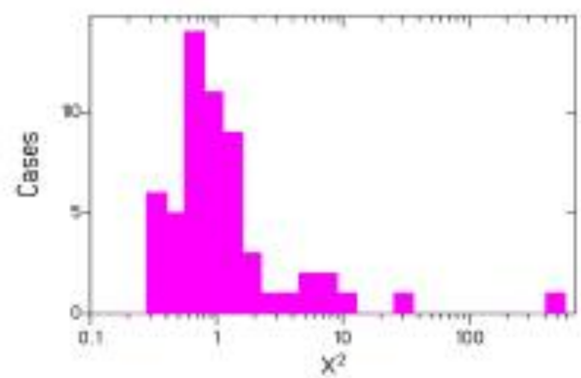



Some deviations around the barrier (structural effects).

# FF mass distributions (sf, 14 MeV)

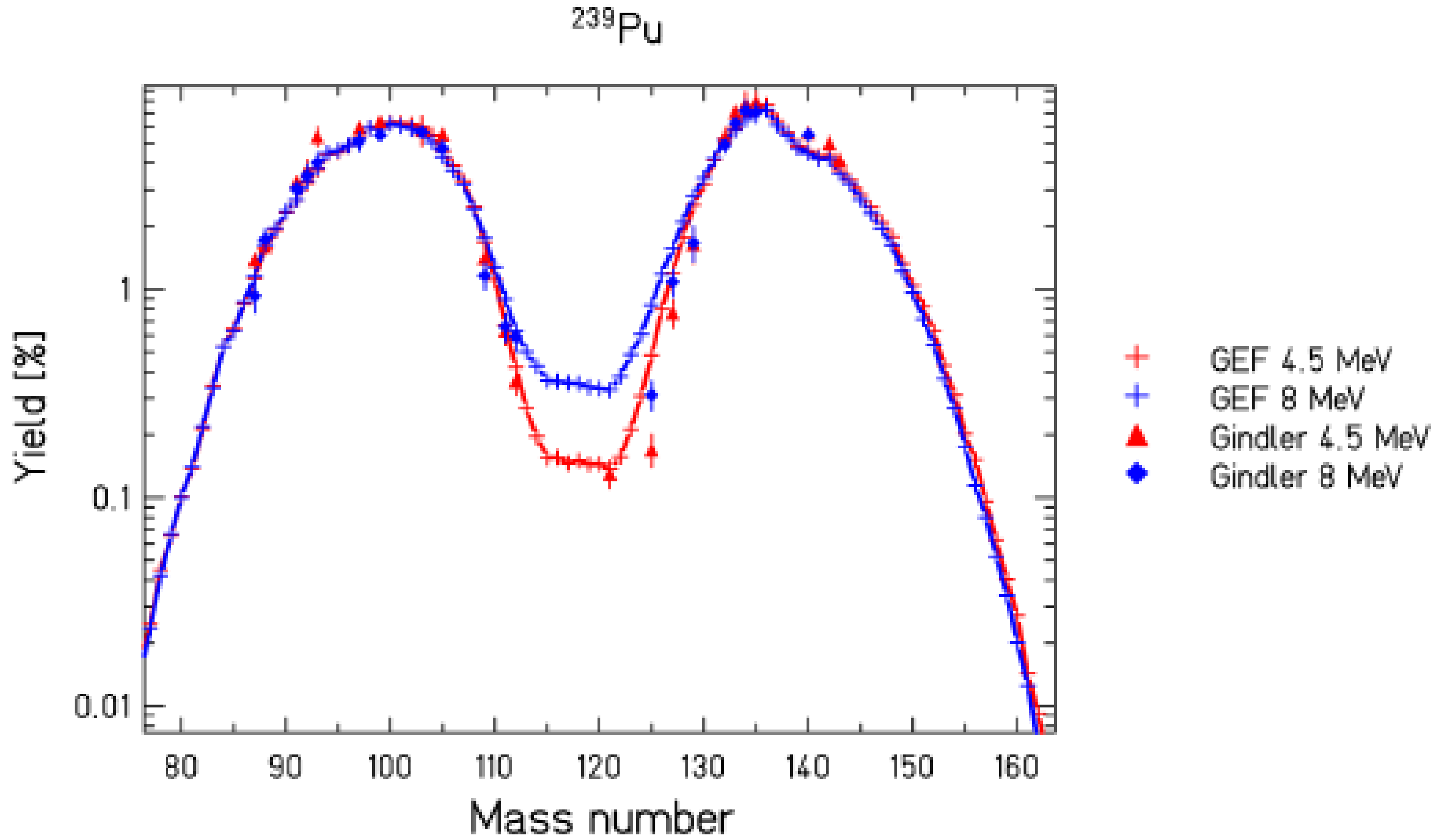



Overall good agreement with ENDF/B-VII

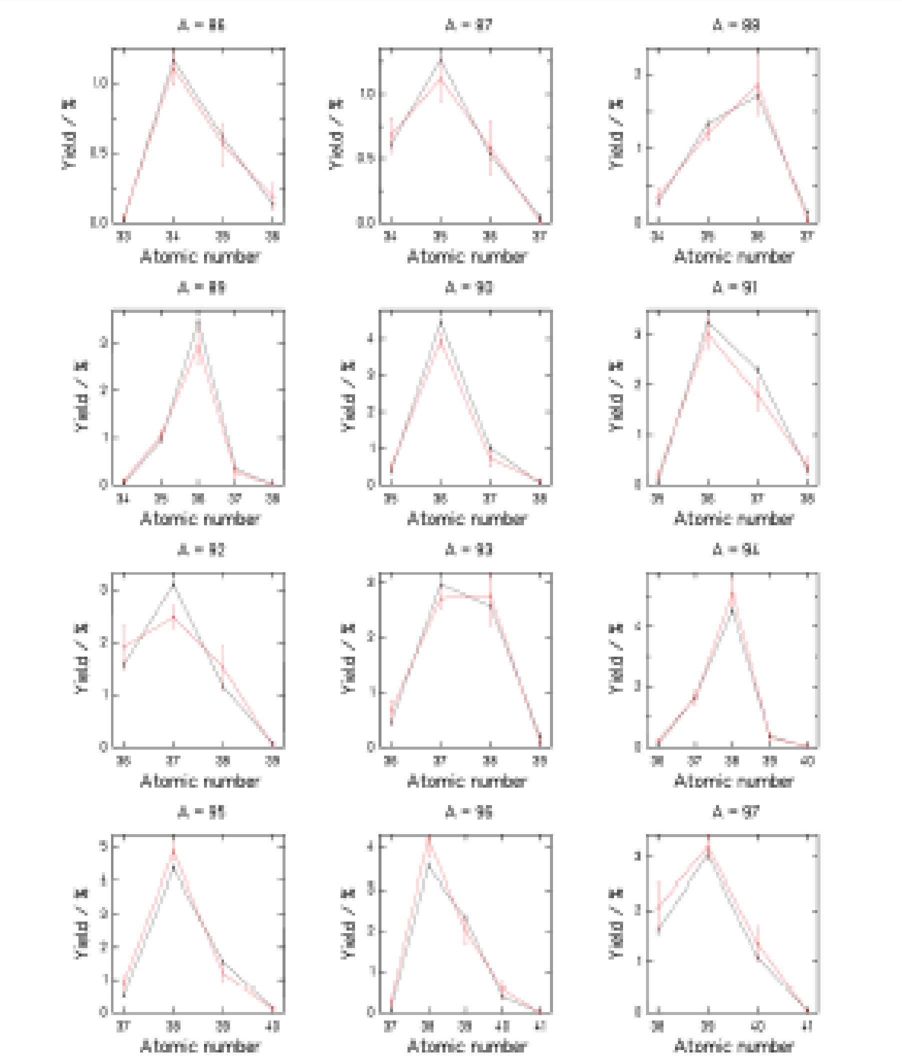
Total: 59 cases

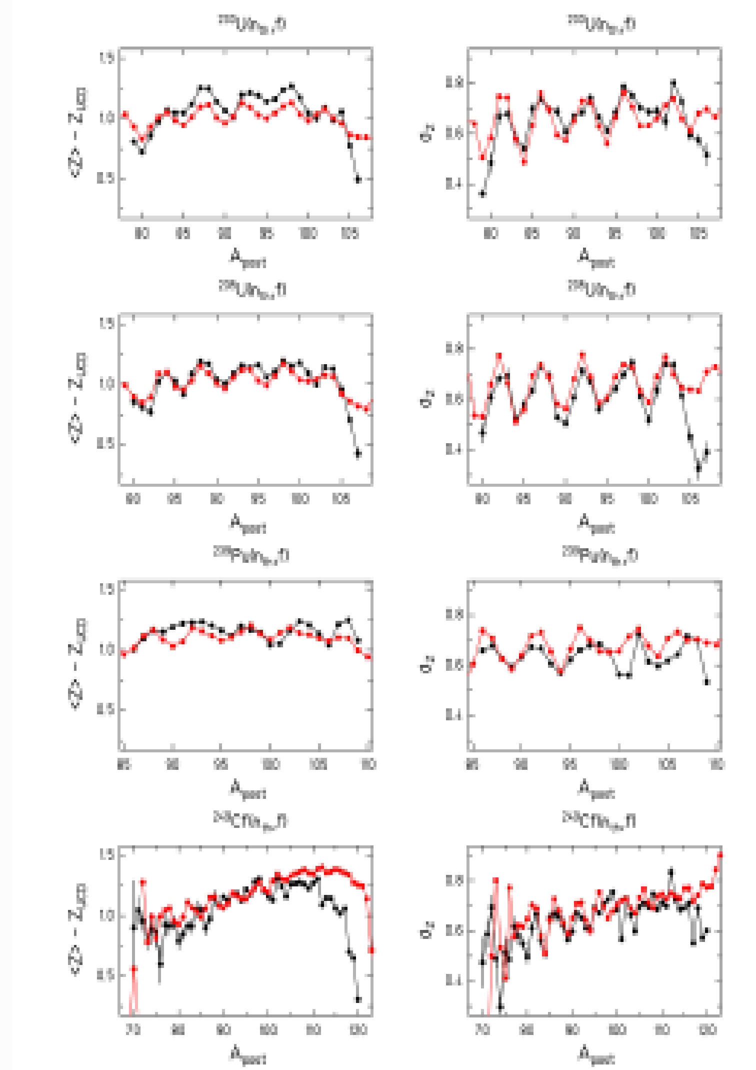
# FF mass distributions (4, 8 MeV)




Data are scarce at intermediate energies.

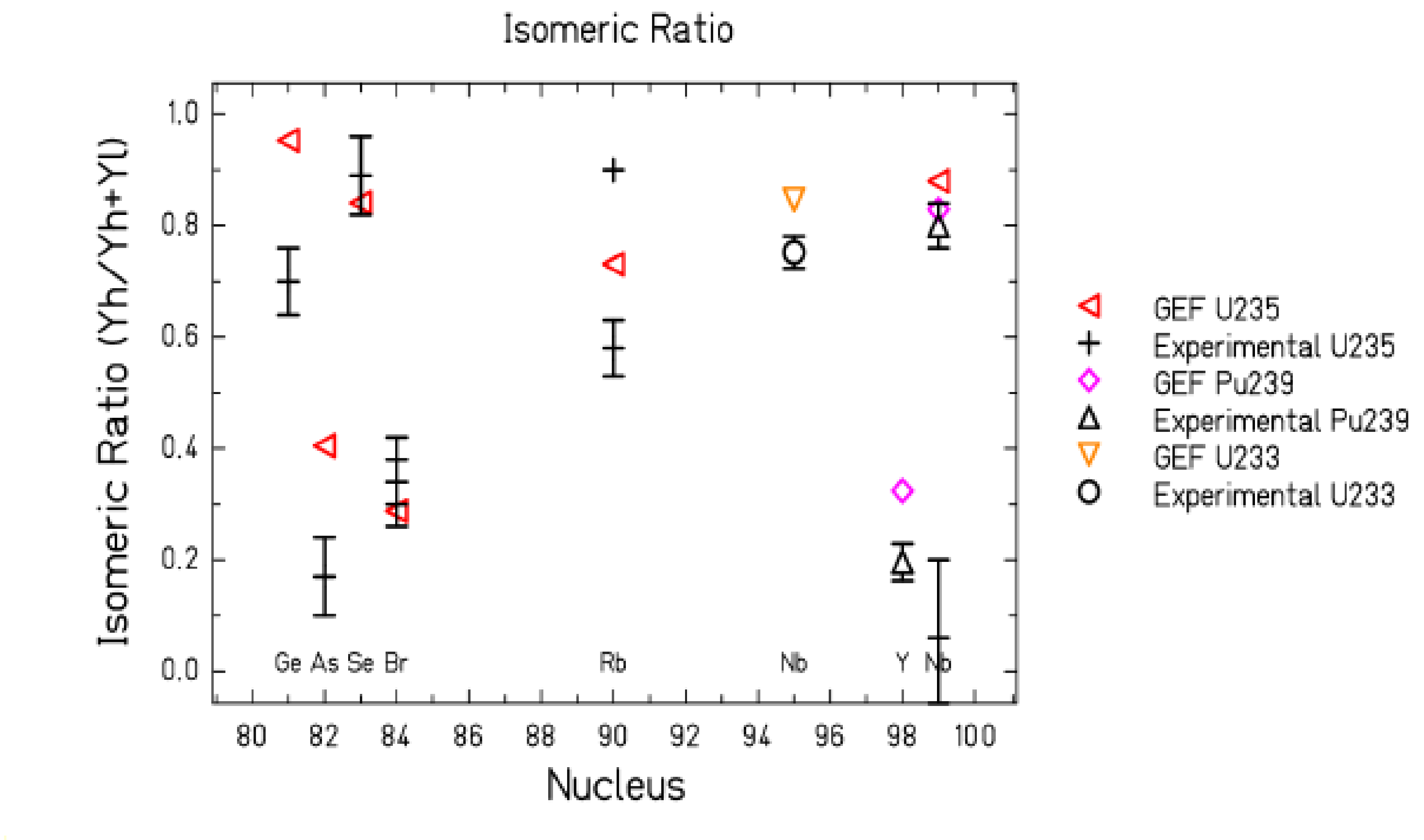
# FF nuclide distributions



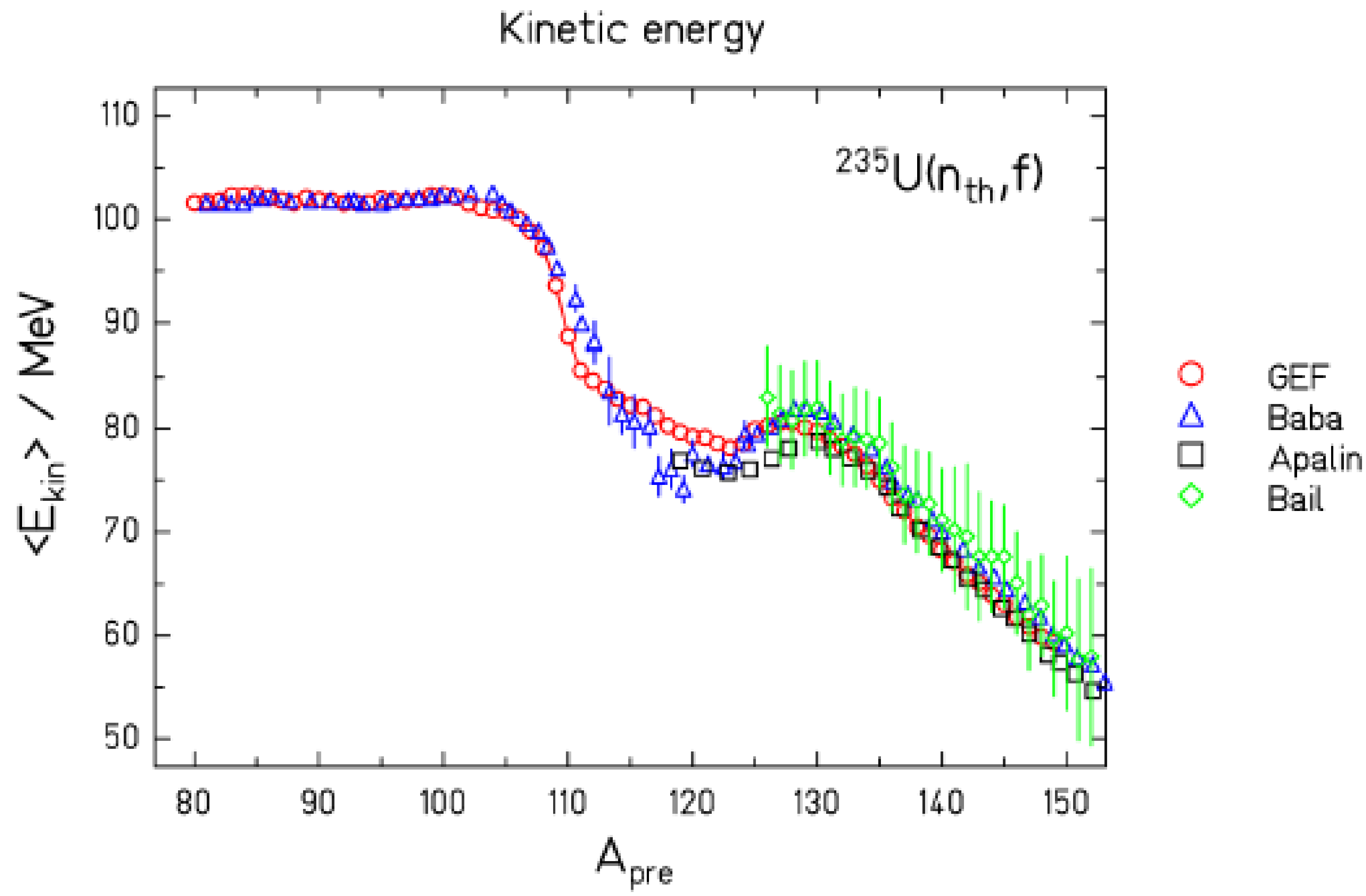




235U(nth,f)

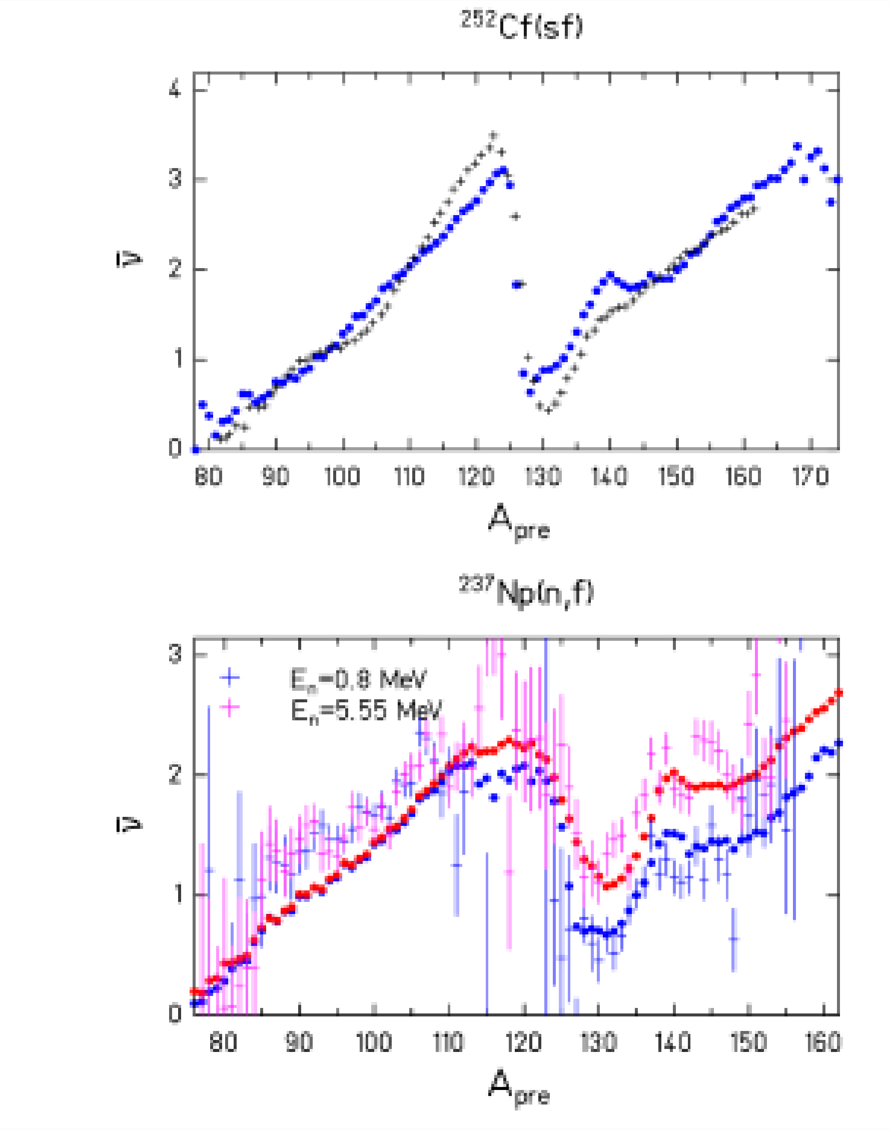
# Isomeric yields



# FF kinetic energies



# nu-bar (A)

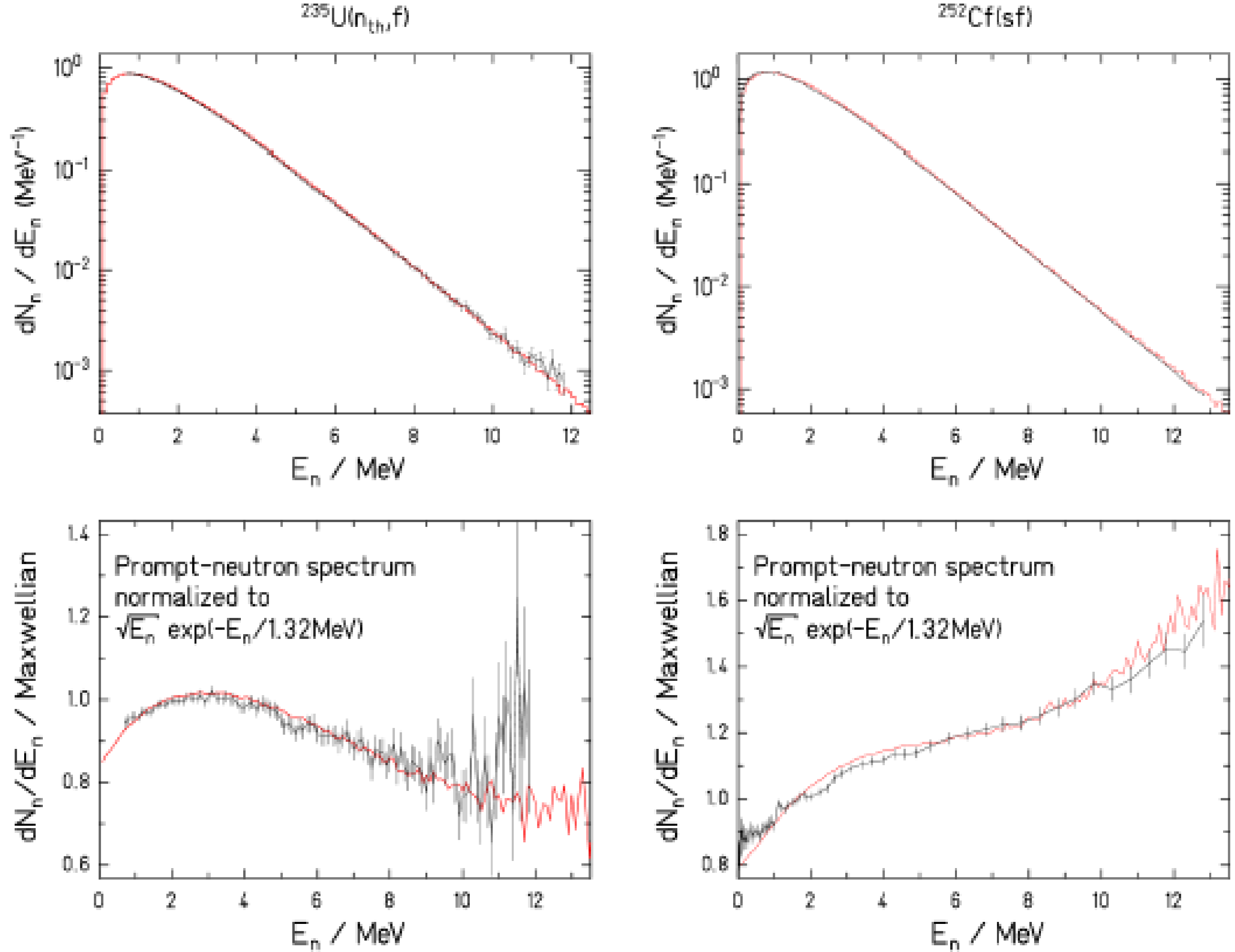



Most important ingredients:

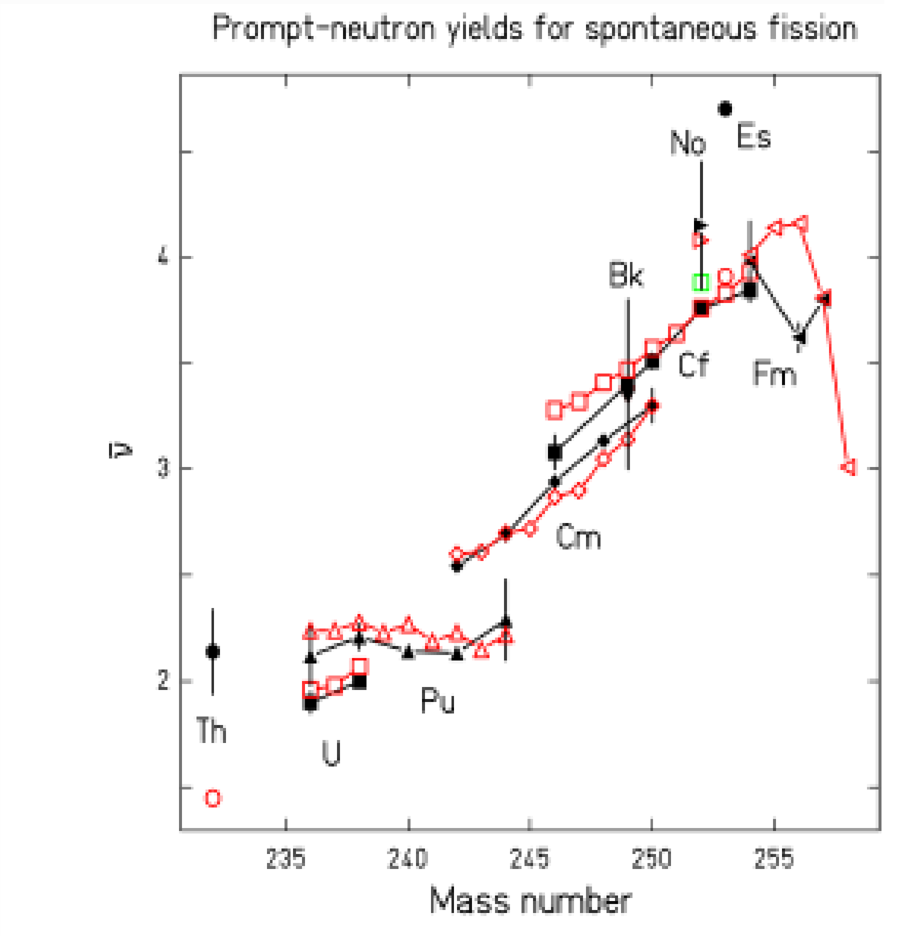
<u>Deformation energy:</u>
Deformation at scission by fragment shells.

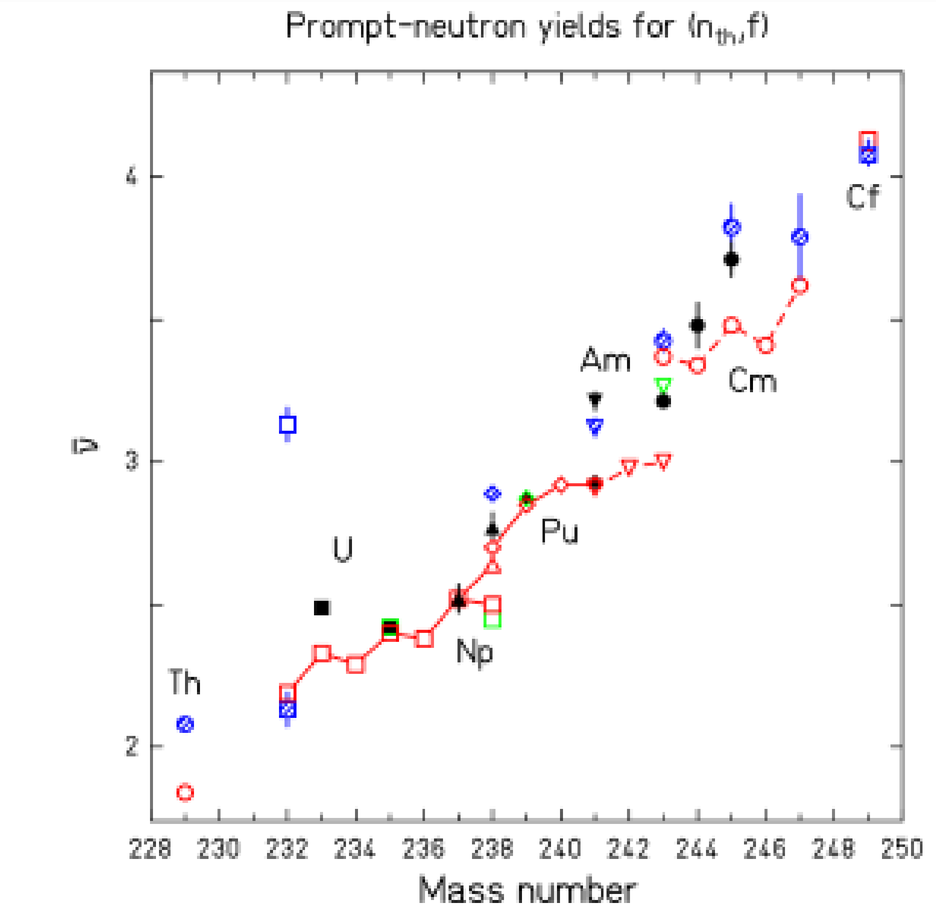
<u>Intrinsic exc. energy:</u>
Entropy-driven energy sorting

# Prompt-neutron spectrum ($n_{th}$, sf)



# nu-bar



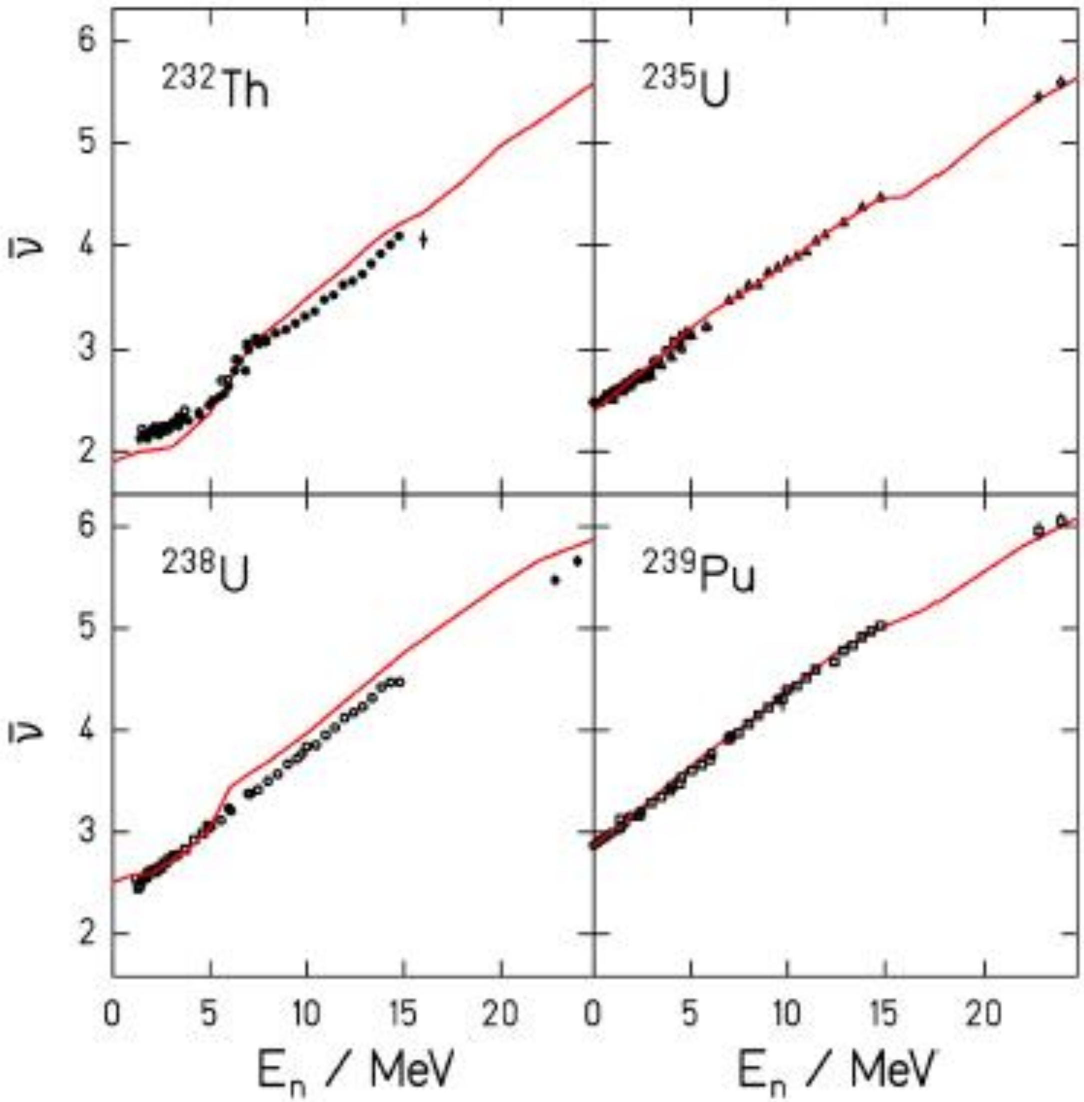




rms deviation: 0.1 units

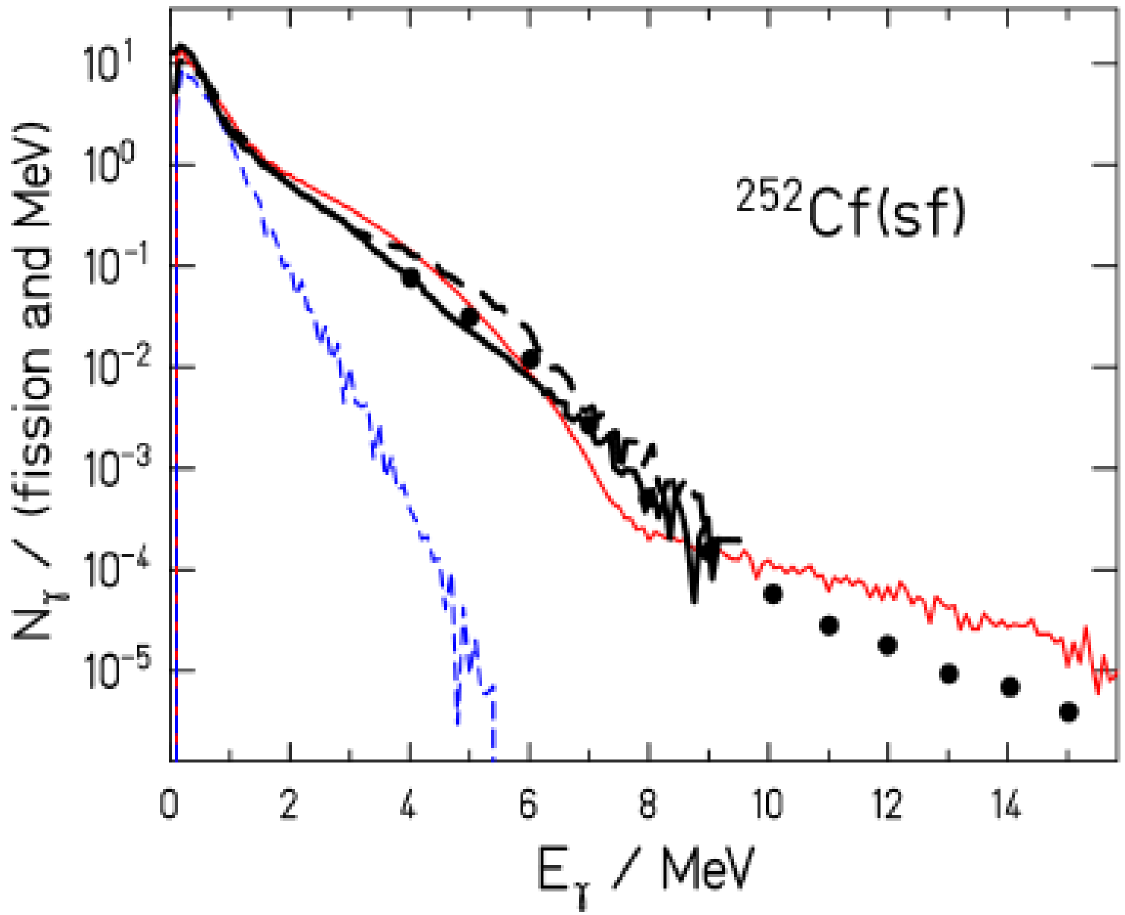
rms deviation: 0.2 units

(experimental problems?)

# nu-bar (E)



# Prompt-gamma spectrum




Experiment

GEF

E2

Measured spectrum: Detector response not unfolded.

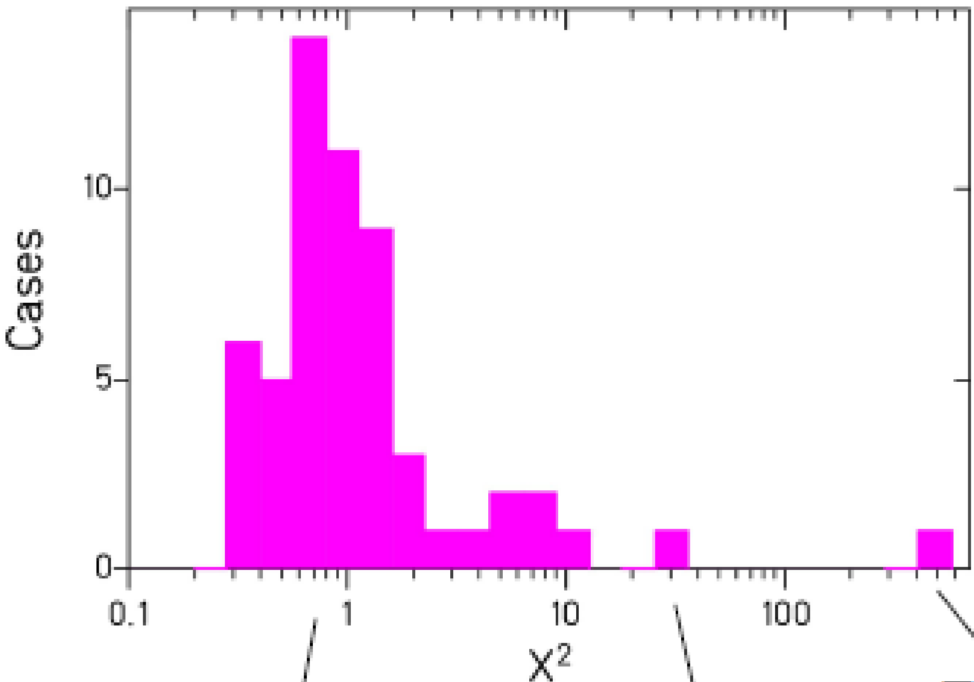
# Conclusion

- GEF covers a large variety of fission observables.
- There is overall good agreement with experiment.
- Most deviations may be attributed to experimental problems.
- A few deviations due to complex structural effects.

# Fundamental virtues and constraints of the GEF model

- Rigid theoretical framework with adjusted parameters.
- About 50 model parameters for several 100 systems + energy variation (far less than 1 parameter per system).
- Predicts the behaviour of a specific system without particular experimental information.
- Cannot be adjusted to a peculiar feature of a specific system.

# Chi-squared deviations of fission yields



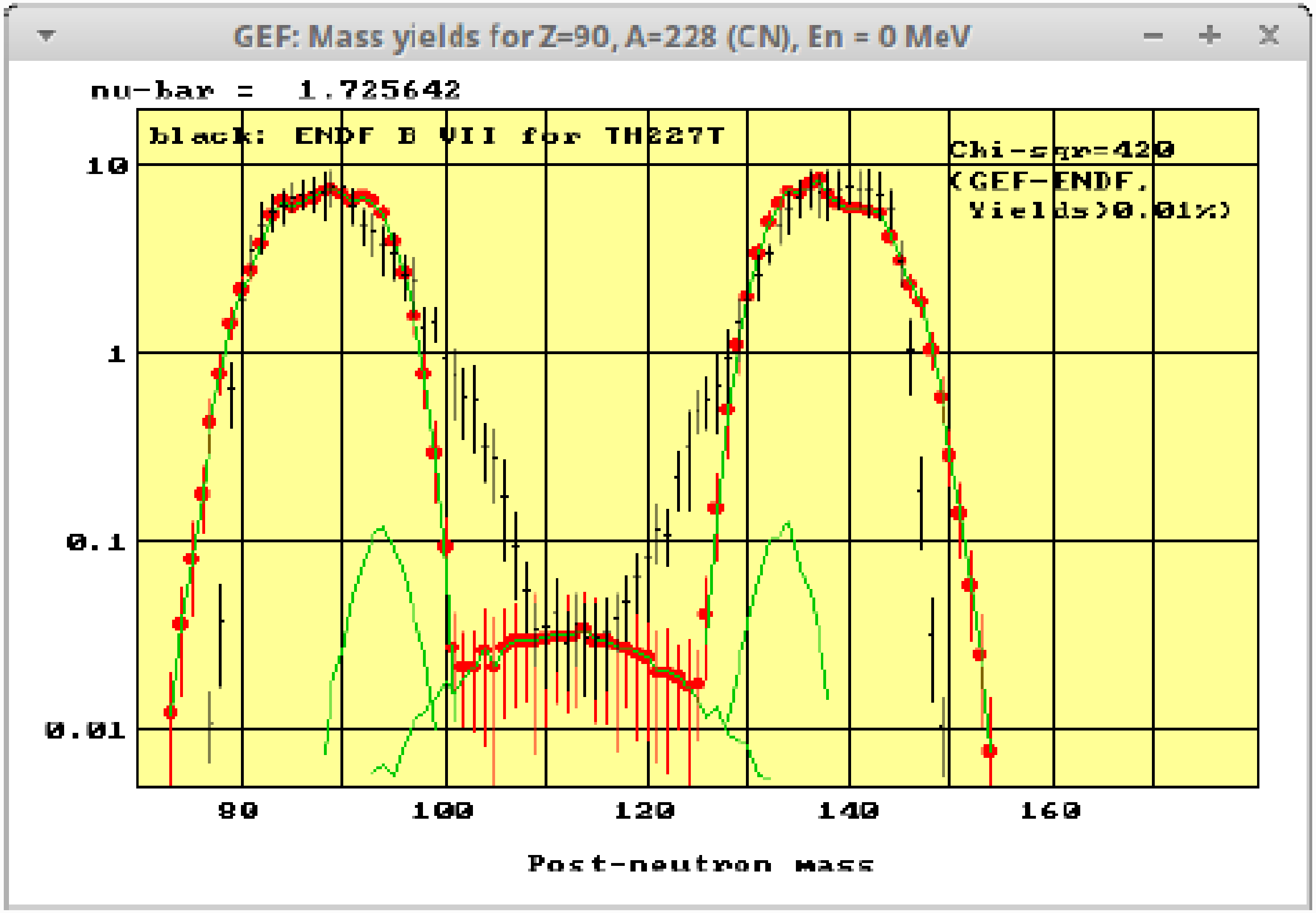

All mass distributions of ENDF/B-VII.

TH227T

TH229T

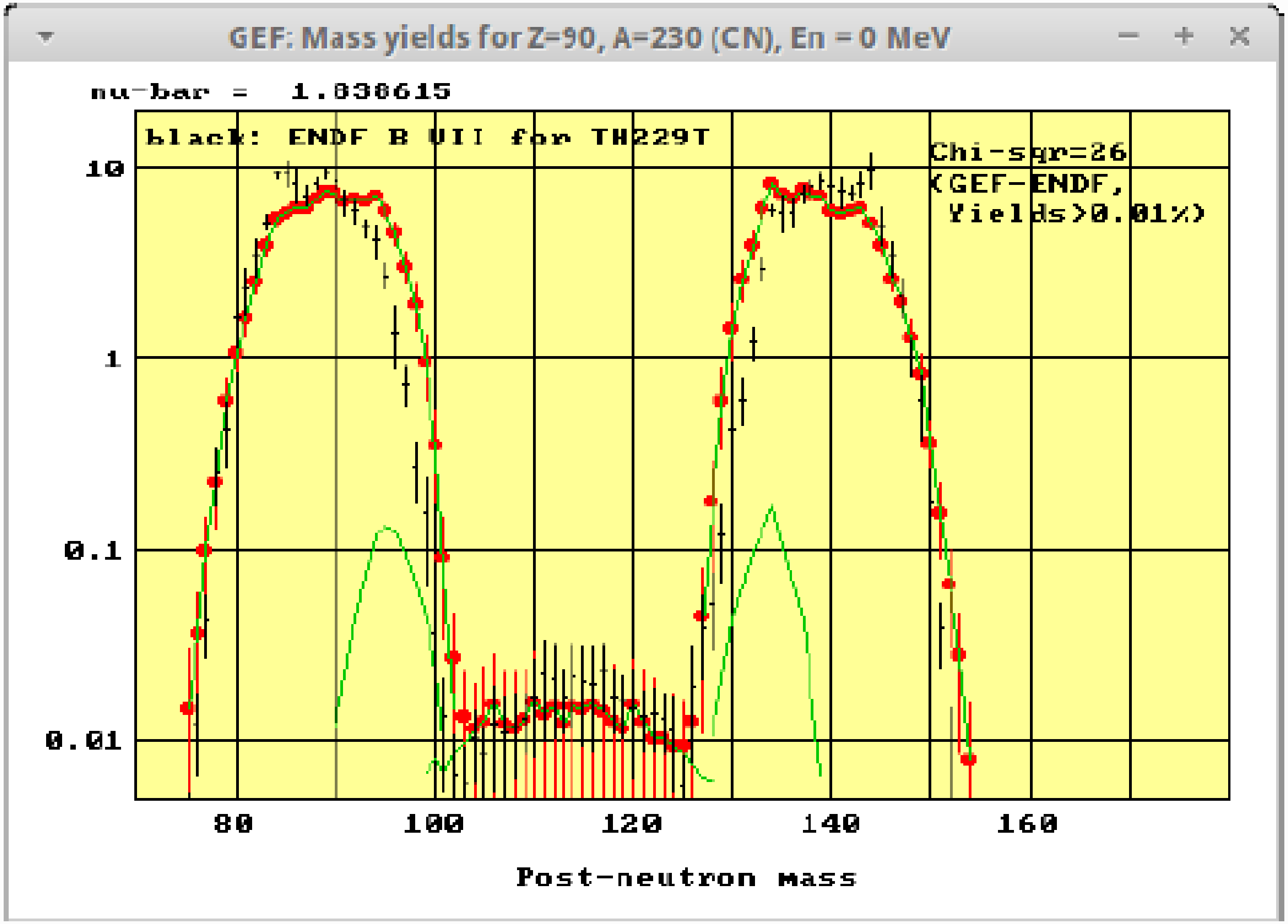
50 of 59 cases
in the peak around 1.
(Deviations do not exceed
experimental uncertainties.)

# TH227T




Chi-squared = 420 !
Probably wrong behaviour of evaluated mass distribution in the wings of the asymmetric peaks.

# TH229T

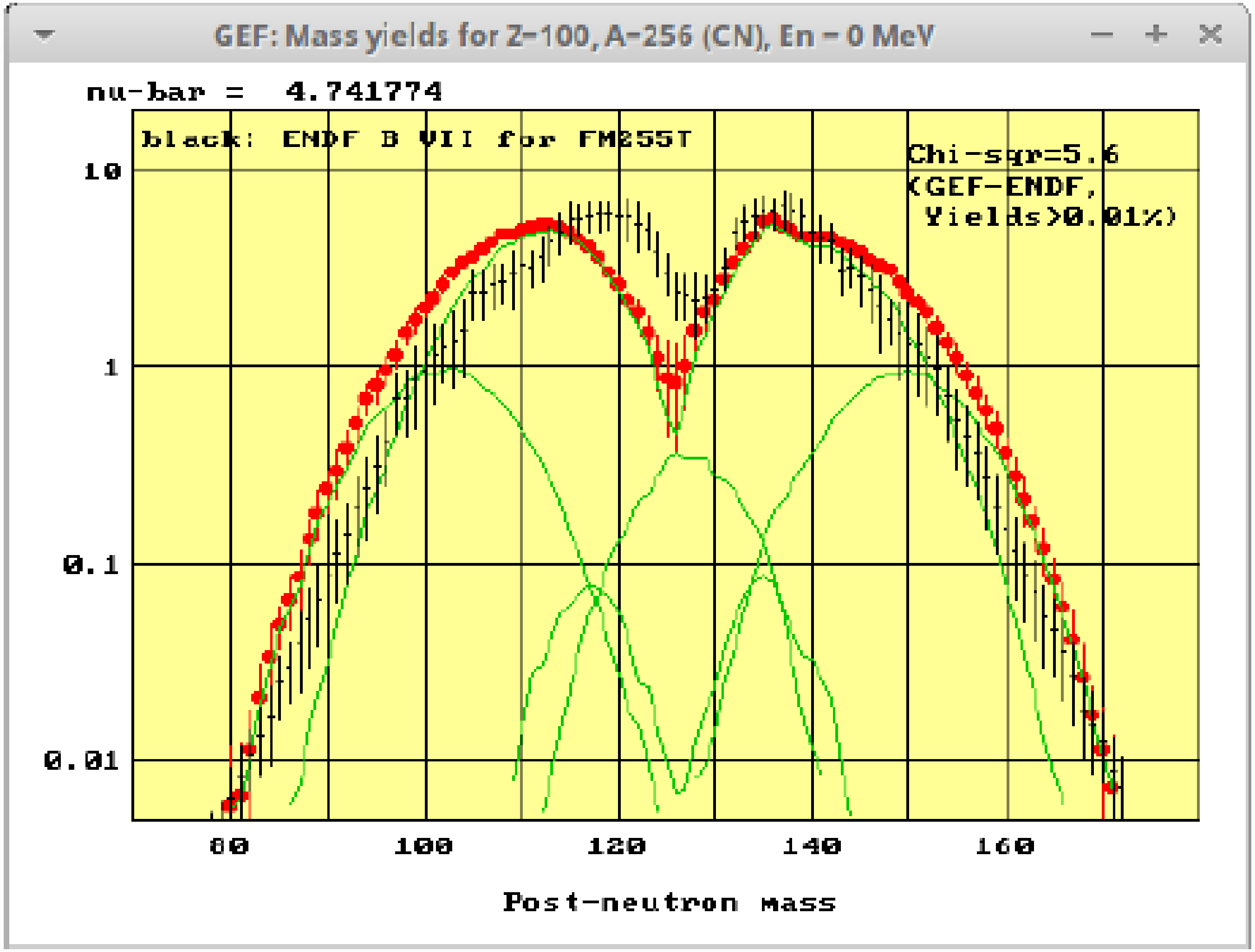



Chi-squared = 26.

Wrong position of inner wing of distribution in GEF.

Only case where GEF is proven to be off!

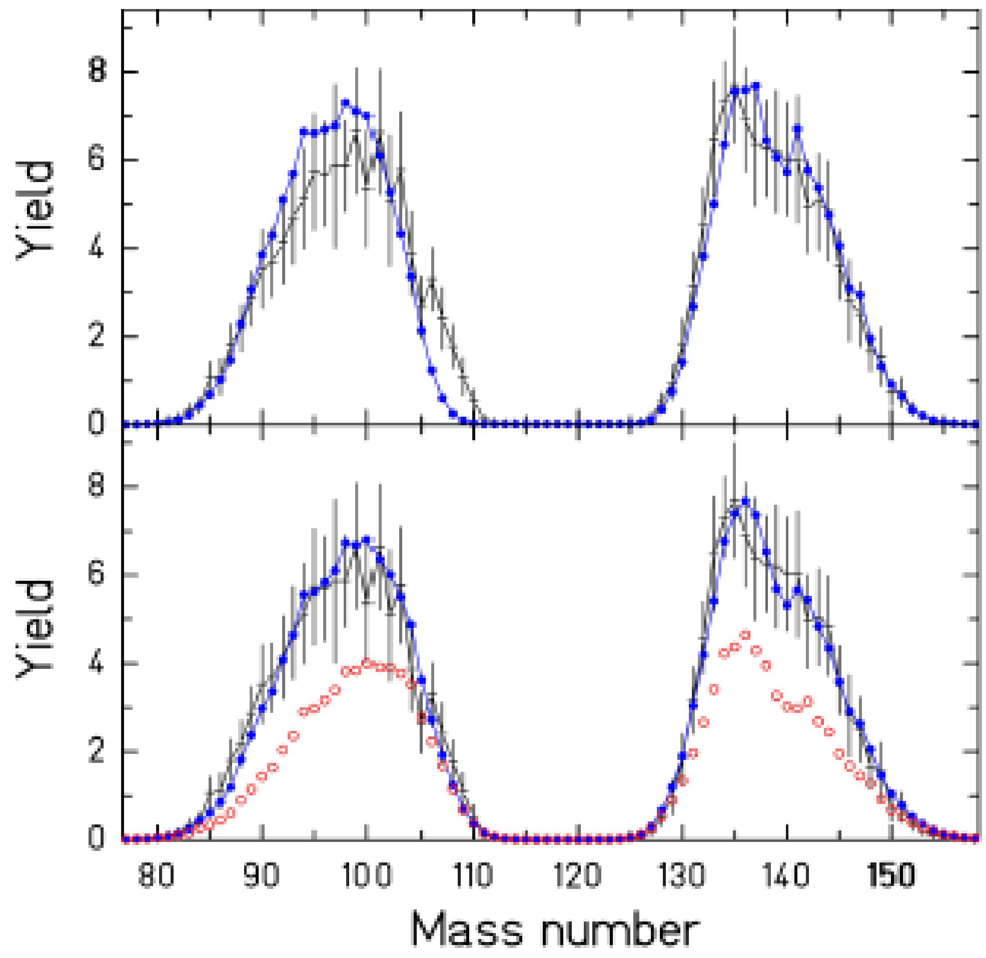
# Fm255T




Chi-squared = 5.6.

Distribution symmetric around A = 128 = A_CN/2 → No room for prompt-neutron emission! (4.74 neutrons expected.)

# Np237T



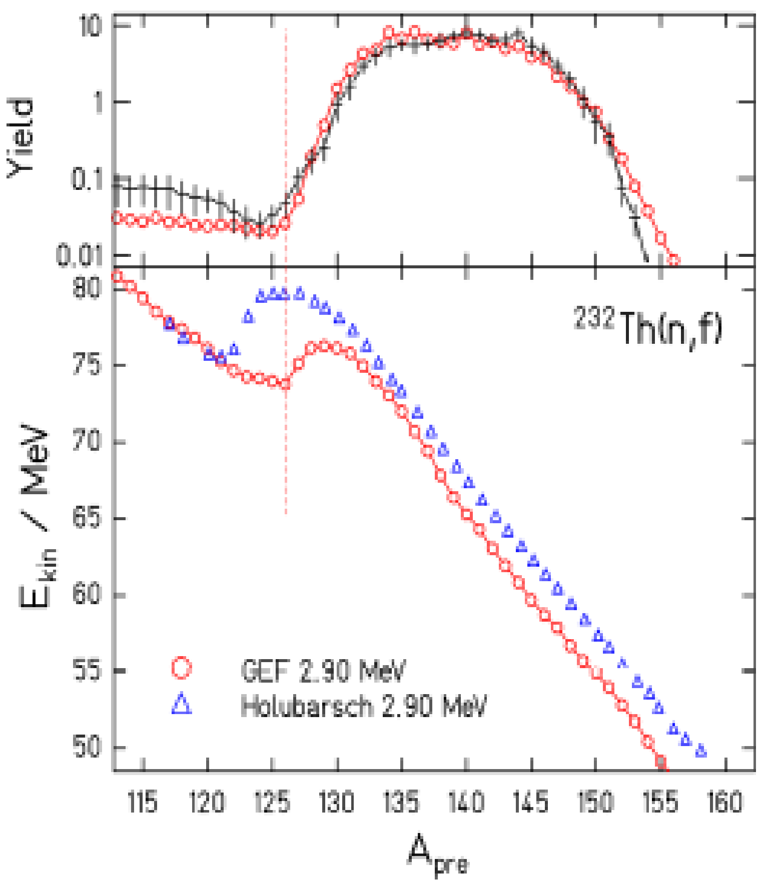

Data: ENDF/B-VII

GEF:
Pure 237Np target

GEF:
40 % 237Np
60 % 239Pu target

Indication for a huge target impurity.

# Ekin for 232Th(n,f)




GEF calculation:
Kink in mass yield and
in Ekin coincide.

Data:
Kink in Ekin is shifted!

→ **Problem in the mass calibration.**

# Conclusion

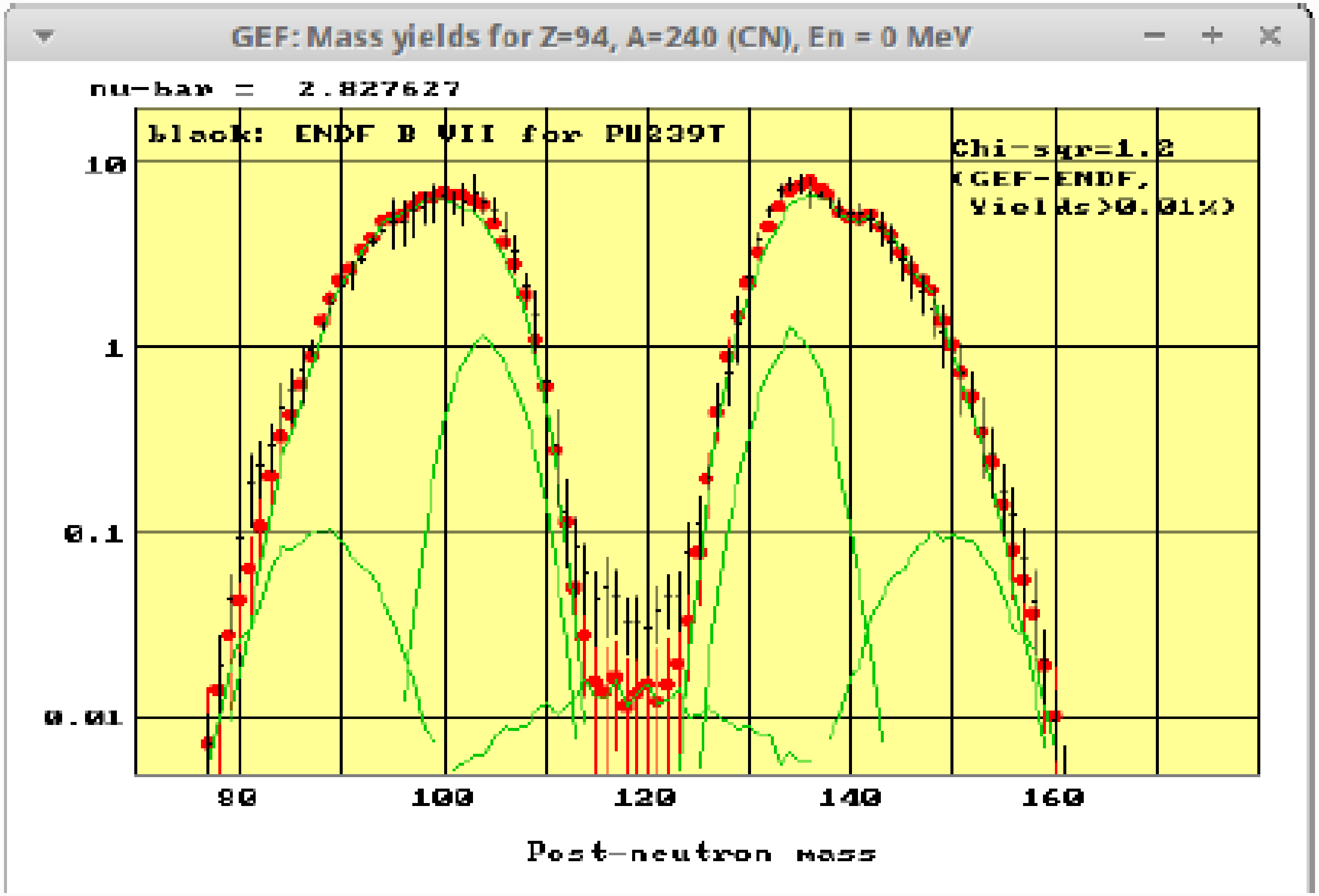
- A systematic comparison of measured data with the results of the GEF code can reveal wrong data and erroneous evaluations.
- The link between different fission observables provided by the GEF model can reveal inconsistencies between different kind of experimental data.
- In general, the GEF code can be a valuable tool for improving the evaluation of nuclear data.
- GEF may also help to better target and to reduce the amount of necessary experiments.

# Fission observables from GEF

- Fission-fragment nuclide distributions (Z,A)
- TKE distributions (Z, A, TKE)
- Fission-fragment angular momenta
- Prompt-neutron multiplicities
- Prompt-neutron spectra
- Prompt-gamma spectra

For spontaneous fission and
neutron-induced fission up to En = 20 MeV.

# Example: Mass distribution (PU239T)




Green lines: Fission channels from GEF

Red points and red error bars: Mass distribution from GEF

Black error bars: ENDF/B-VII

Principle parameters (given by the model, simplified):
<A>, sigma_A, Y(A) of each fission channel determined by position, width, depth of the fission valleys (12 parameters).

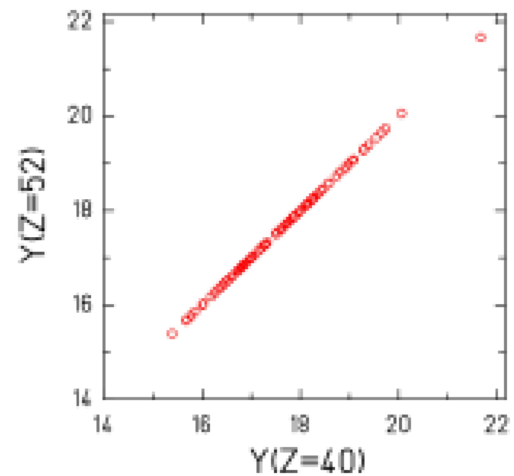
# Uncertainties and covariances

- Calculations with perturbed parameters.
- Unavoidable coupling between the parameters by normalization of yields to 200 %.
- Best values and uncertainties of parameters from CHI-squared of all systems.
- Resulting multi-variant distributions (distributions of mass yields Y(A1) vs. Y(A2)).
- Deduce uncertainties and covariances.

$$\mathrm{cov}(x, y) = \sum_{i=1}^{N} \frac{(x_i - \bar{x})(y_i - \bar{y})}{N}$$

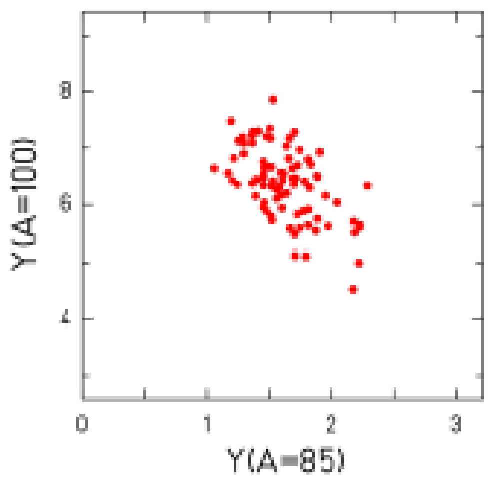
# Multivariant distributions - Typical cases

- relations required by physics




Two complementary elements (Strictly correlated)

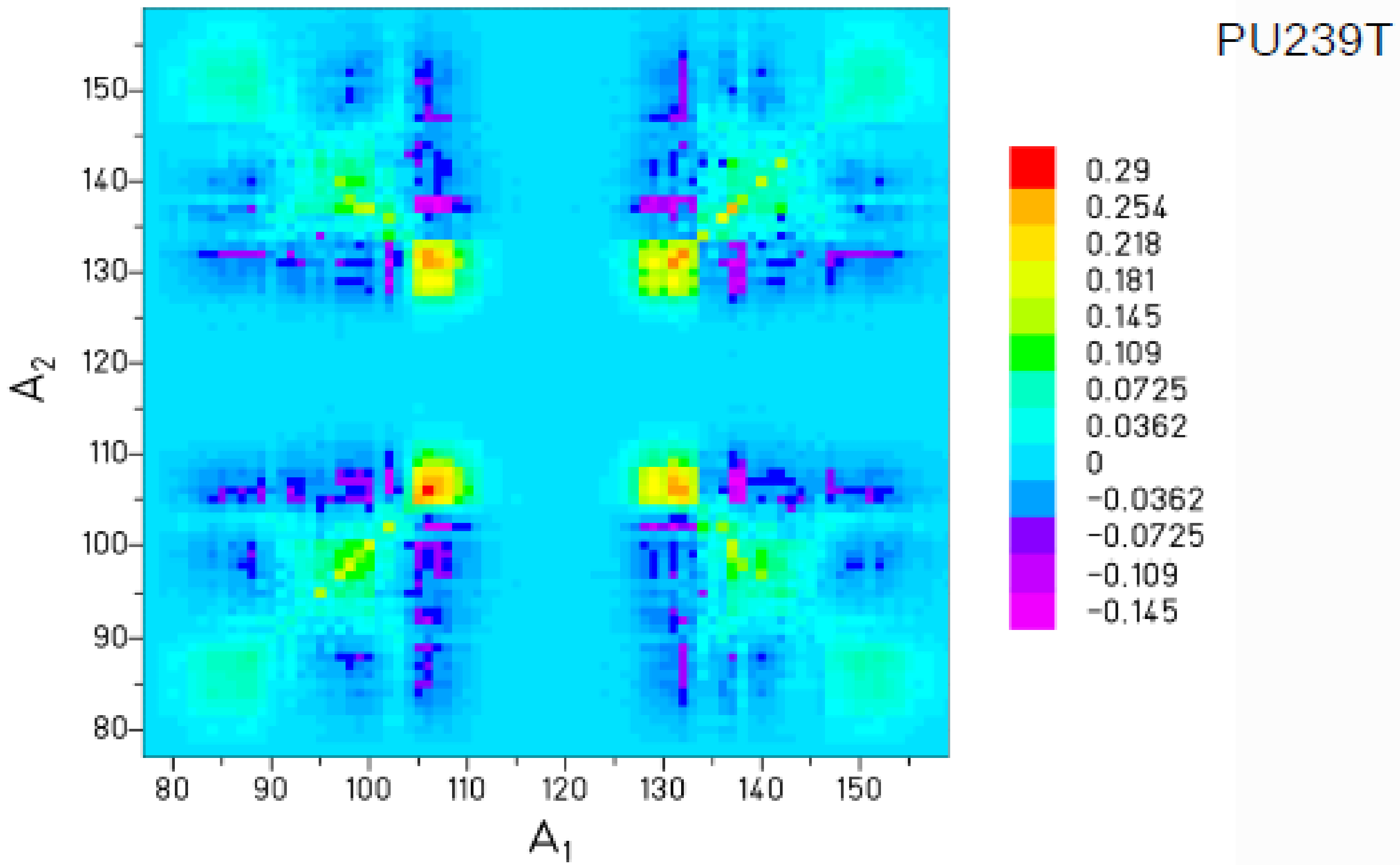
- relations required by the model




Two masses from different modes. (Slightly anti-correlated)

Result of perturbed GEF calculations for 235U(nth,f)

# Full covariance matrix




Determined by the inner logic of the model.
Basically different from experimental covariances!

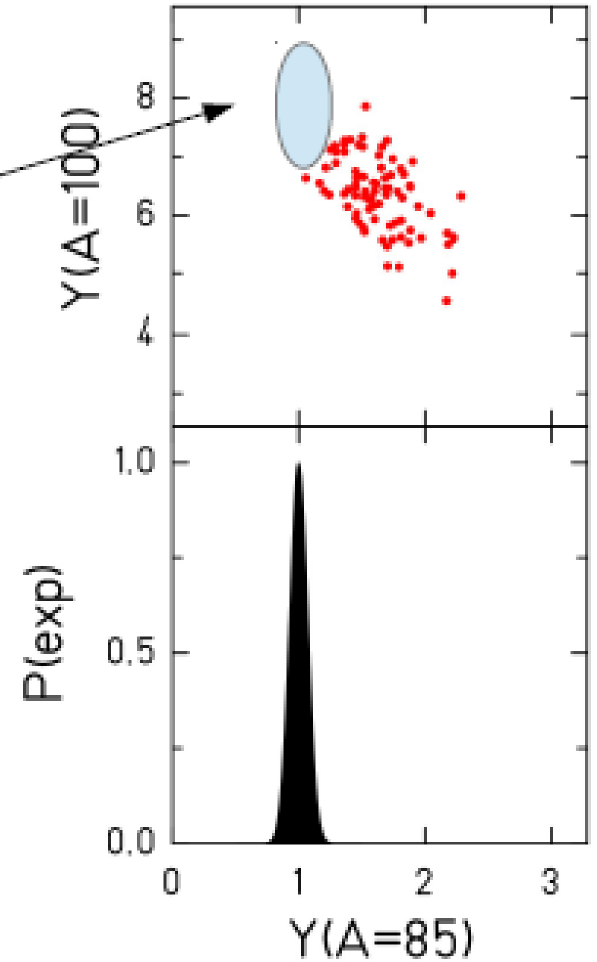
# Combining GEF with experiment (schematic)

GEF result (2 parameters):

Adjusted GEF result:

Experiment (1 parameter):

Discrepancy between model and experiment leads to modification of other GEF results.
Modified GEF results are consistent with experiment.



# Mathematical procedure

- Covariance matrix defines multivariant normal distribution *f* of yields compatible with GEF:

$$f = \frac{1}{(2\pi)^{k/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\bar{\mathbf{x}})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\bar{\mathbf{x}})\right)$$

covariance matrix yields

- Log-Likelihood function derived from GEF:

$$L_{GEF} = \ln(f)$$

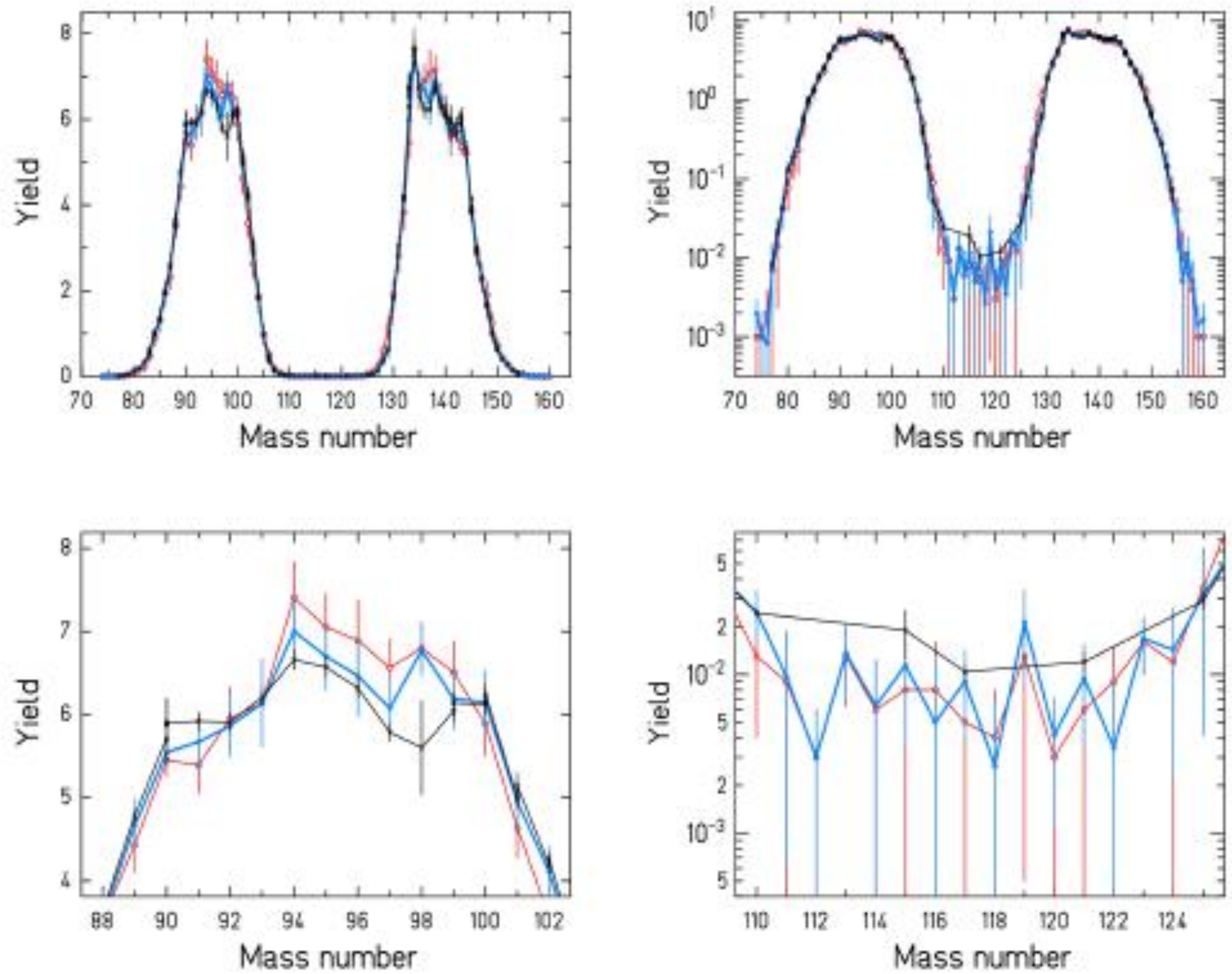
- Same procedure for experimental data → $L_{exp}$
- Combined: $L_c = W_{GEF}\, L_{GEF} + W_{exp}\, L_{exp}$ ($W \approx 1/N$)
- Determine yields by searching max($L_c$)
- Result: Adjusted (completed) set of yields.

# Dedicated code for search of maximum likelihood

- MATCH code
- Combines experimental data (incomplete, subject to uncertainties) with the prediction of the GEF code.

# Example 1

U235T



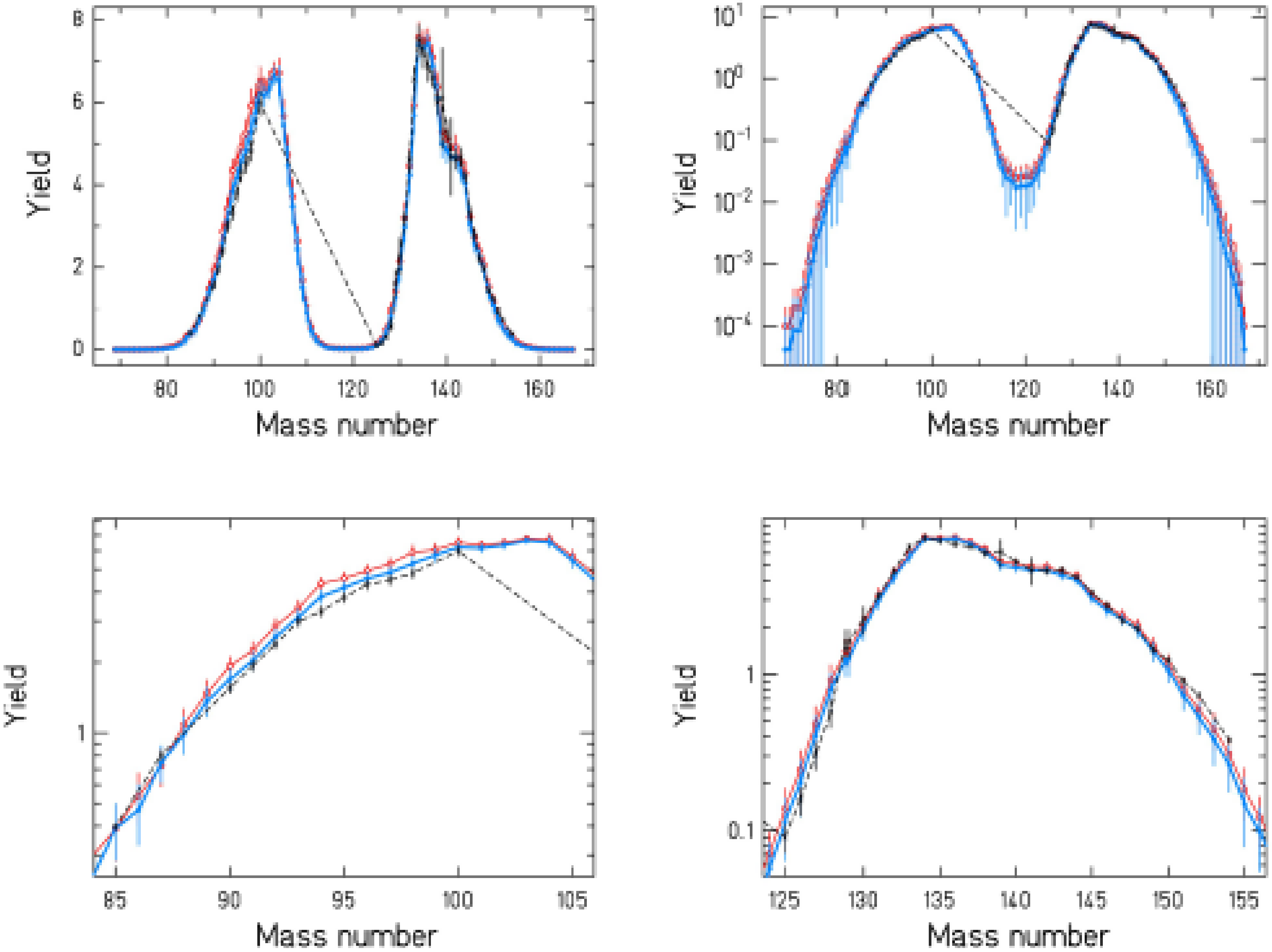

Data

GEF

MATCH

# Example 2

Pu241F




Data

GEF

MATCH

# Conclusion

- GEF code produces covariances between any pairs of fission data.
- Covariances are defined by the physics of the model.
- Combining Log(likelihood) of model and experiment provides the best compromise.
- Fine tuning of the model and/or guess of incomplete data.
- Optimisation performed by the MATCH code.

Codes: GEF and MATCH from www.khs-erzhausen.de

# Problem of weighting

- **Equivalent weighting (GEF and experimental)**
  - Absolute values and correlations of GEF considered
    Pro: GEF model is adjusted to a large body of experimental data. Besides the correlations, the absolute results of GEF should have some weight for the evaluation.

- **What is equivalent weighting?**
  - If correlations are similar in GEF and experiment
    → weighting by number of data points

- **Dominant weighting of experimental data**
  - Experimental data are not modified
  - Correlations of GEF still used to "adjust" GEF results
    Pro: "Objective" experimental data should not be "spoiled" by "subjective" model predictions.