General description of fission observables: The GEF code*

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Invited plenary talk

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Different approaches for modeling fission

↑ fundamental

- Fully microscopic, self-consistent models
- Stochastic models (Langevin equations)
- Semi-empirical description of the properties and processes of the fissioning system (GEF)
- Empirical parametrization of the fission observables (Wahl, Katakura, …)

↓ parametrization

GEF compared to direct parametrization of observables

GEF	Empirical parametrization
1. Rigid theoretical frame • Universal fragment shells • Topographic theorem • Energy sorting, etc.	1. No theoretical input
2. Global description of all systems, E*, spin	2. Separate description of individual systems
3. All fission quantities and observables	3. Only specific observables
4. Each fission quantity correlates with all others	4. Separate description of different observables
5. Multi-chance fission	5. Lumped observables

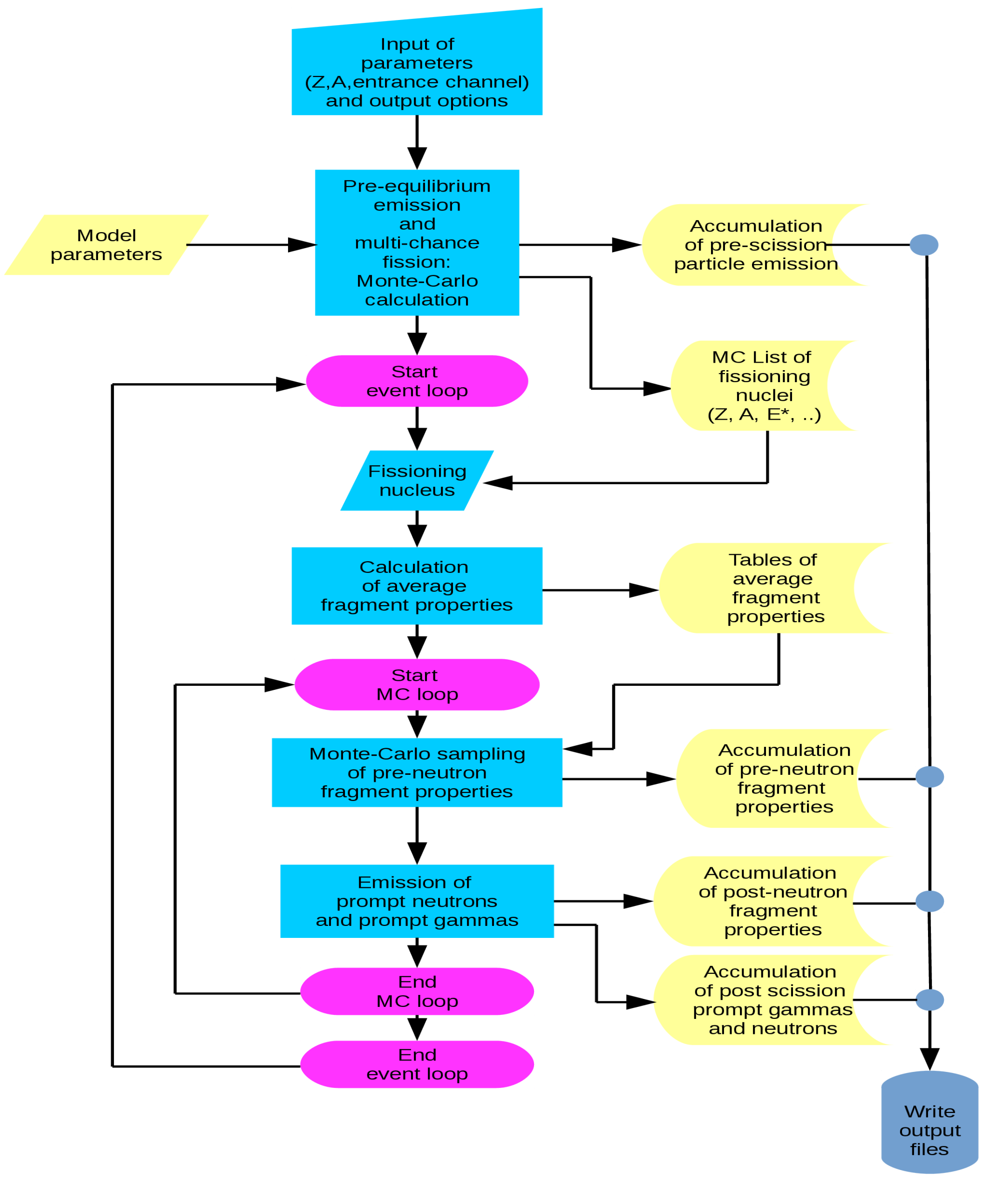
Theoretical ideas exploited in GEF

- "Structure of the potential energy surface at large deformations" (Early manifestation of fragment shells), U. Mosel, D. Scharnweber, Phys. Rev. Lett. 25 (1970) 678
- "Theory of macroscopic fission dynamics" (Dynamical freezing), G. D. Adeev, V. V. Pashkevich, Nucl. Phys. A 502 (1989) 405
- "Nuclear properties according to the Thomas-Fermi model" (Topographic theorem), W. D. Myers, W. J. Swiatecki, Nucl. Phys. A 601 (1996) 141

Specific theoretical developments for GEF

- "Assessment of saddle-point-mass predictions for astrophysical applications", A Kelic, K.-H. Schmidt, Phys. Lett. B 634 (2006) 362
- "On the topographical properties of fission barriers", A. V. Karpov, A. Kelic, K.-H. Schmidt, J. Phys. G: Nucl. Part. Phys. 35 (2008) 035104
- "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
- "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 83 (2011) 014607
- "Final excitation energy of fission fragments", K.-H. Schmidt, B. Jurado, Phys. Rev. C 83 (2011) 061601(R)
- "Inconsistencies in the description of pairing effects in nuclear level densities", K.-H. Schmidt, B. Jurado, Phys. Rev. C 86 (2012) 044322
- "General laws of quantum and statistical mechanics governing fission", K.-H. Schmidt, B. Jurado, FIAS Interdisciplinary Science Series (2014) 121
- "Influence of complete energy sorting on the characteristics of the odd-even effect in fission-fragment element distributions", B. Jurado, K.-H. Schmidt, J. Phys. G 42 (2015) 055101
- "Revealing hidden regularities with a general approach to fission", K.-H. Schmidt, B. Jurado, Eur. Phys. J. A 51 (2015) 176

Structure of the GEF model code



Input:

- n-induced fission: En, target
  - Pre-equilibrium
  - Multi-chance

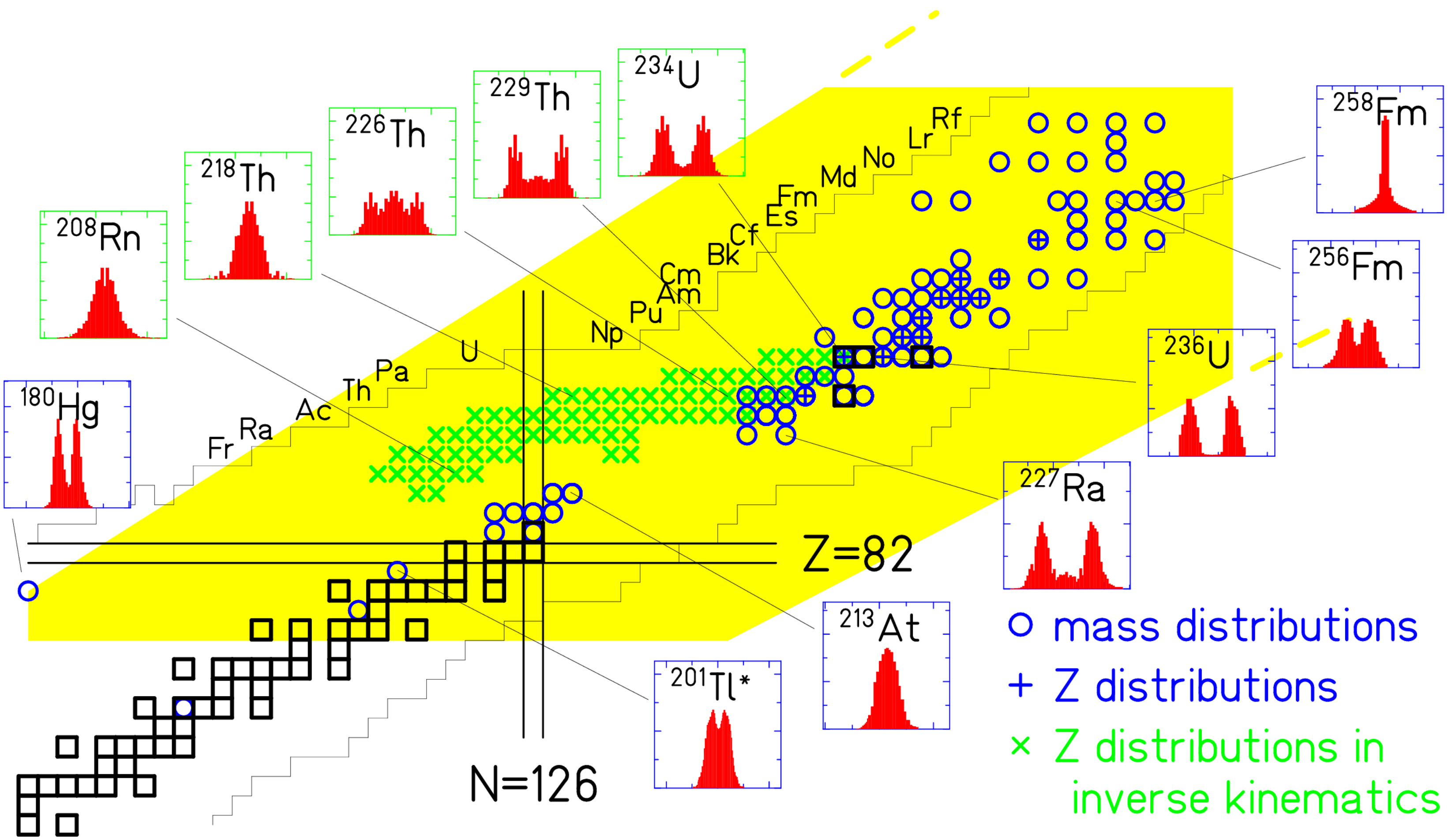
or

- Z, A, E*, I of CN

Output:

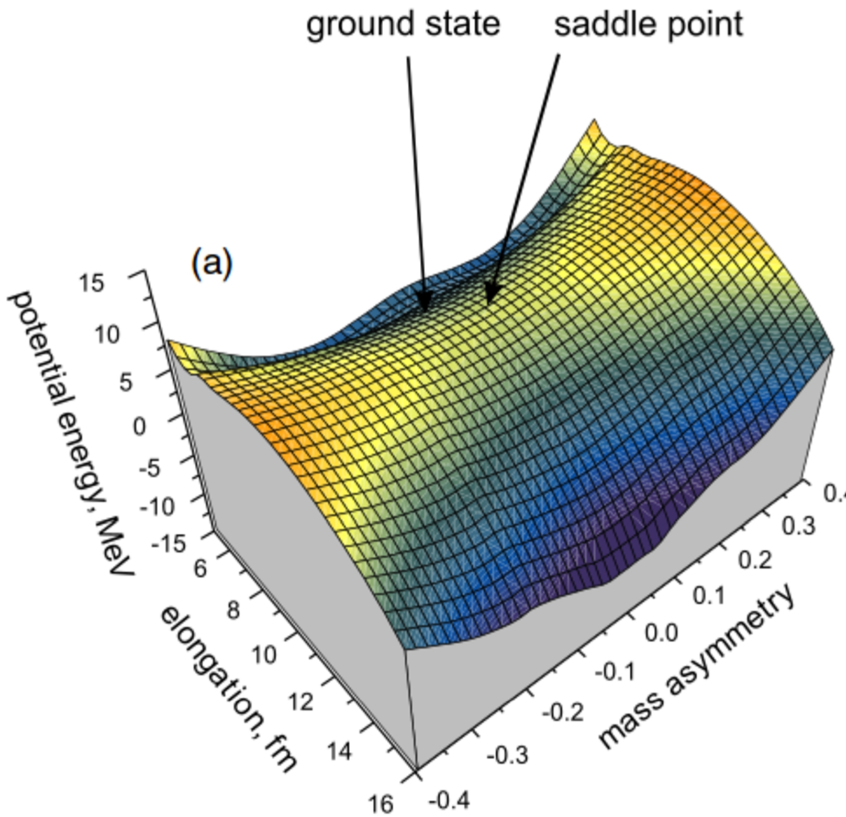
- Z1, A1, Z2, A2,, I1,I2, pre-and post-neutron, isomeric ratios, TKE, prompt neutrons and gammas
- Event generator, covariances, ENDF files, random files

Application range of GEF

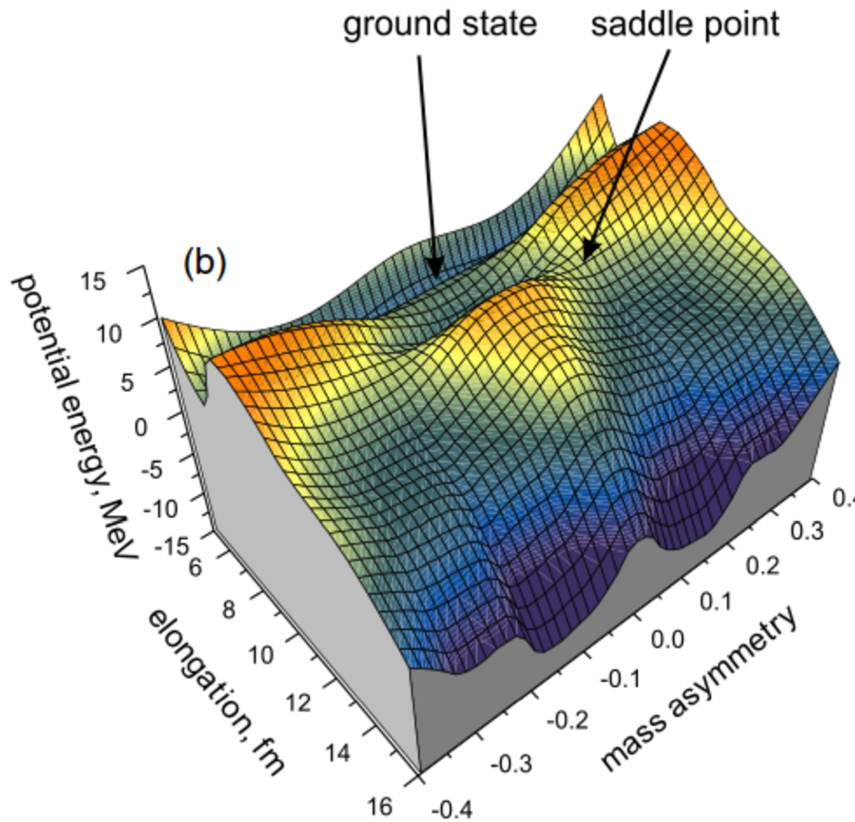


All systems (spontaneous fission up to E*=100 MeV) with a unique parameter set, ≈ 30 to 50 parameters relevant for FY.

Physics of GEF: Potential-energy surface - macro-microscopic approach



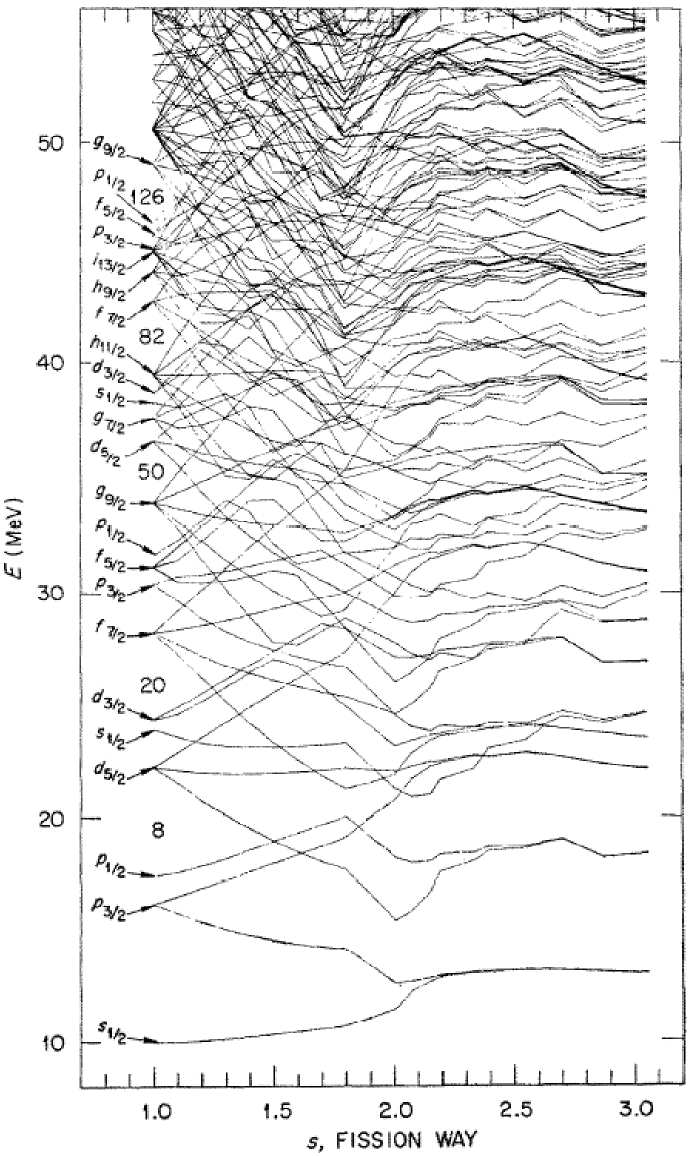
Macroscopic potential



Full potential

A. V. Karpov, A. Kelic, K.-H. Schmidt
J. Phys. G: Nucl. Part. Phys. 35 (2008) 035104

Early influence of fragment shells

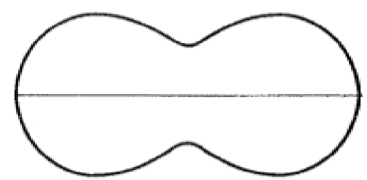


Ground state

Second barrier

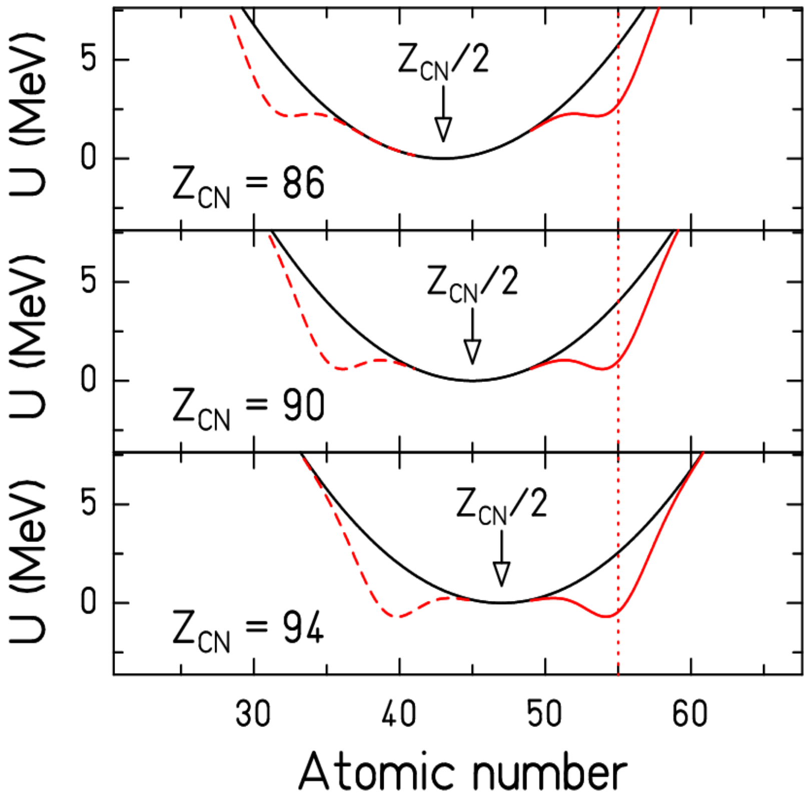
Scission

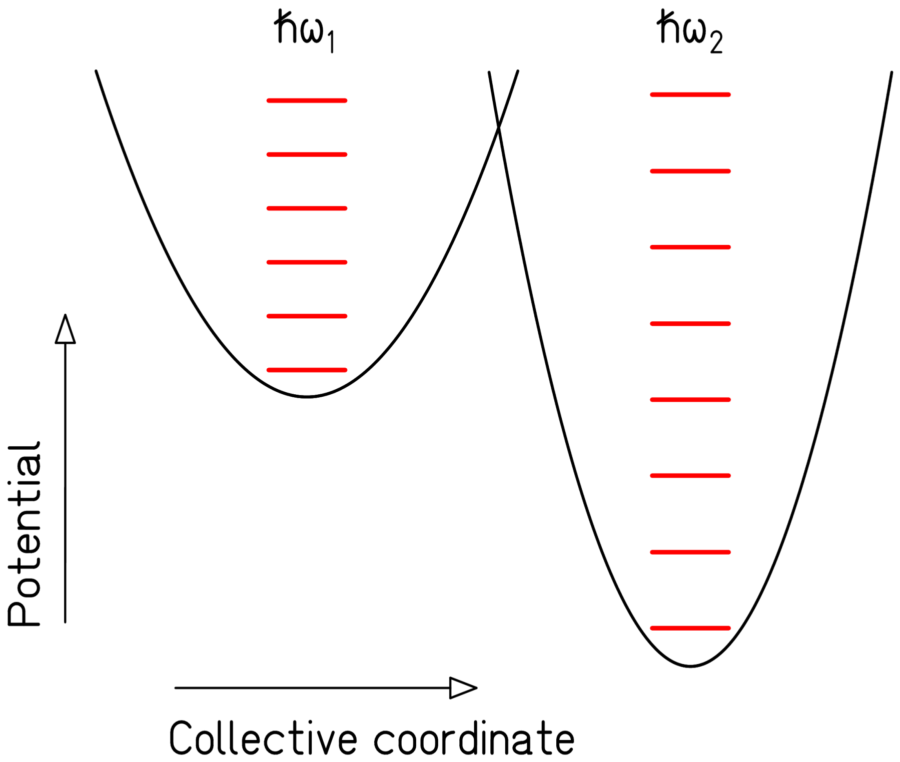
Neutron shell-model states in 2-center shell model (U. Mosel, H. W. Schmitt, Nucl. Phys. A 165 (1971) 73)



- Single-particle levels near second barrier resemble those of separated fragments.
- Quantum-mechanical effect of necked-in shape.

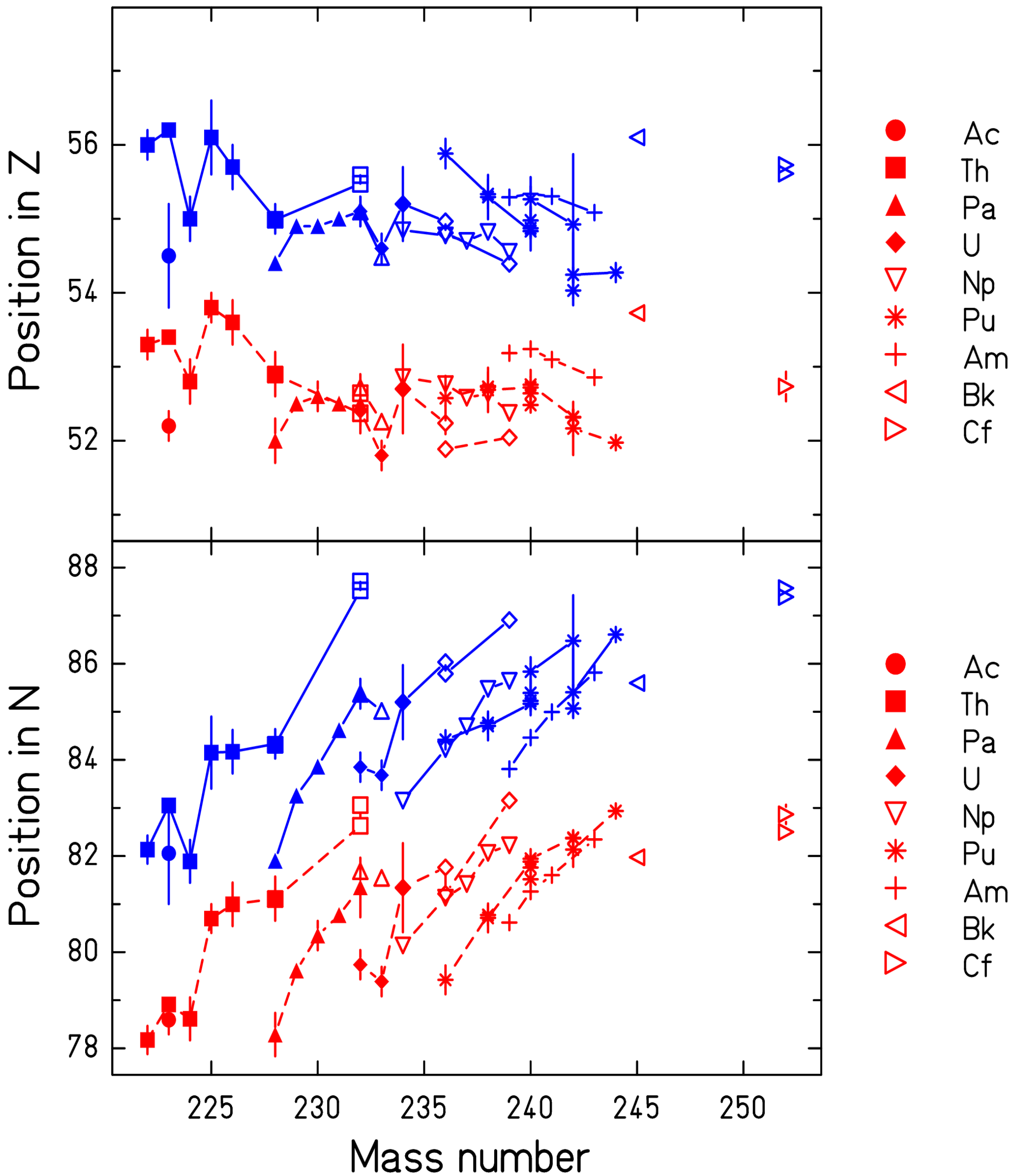
Physics of GEF: Separability of (CN) macroscopic potential and (fragment) shells





Statistical population of quantum oscillators in asymmetry:
Yield and shape of fission channels

Empirical parameters of fragment shells



Böckstiegel et al., 2008

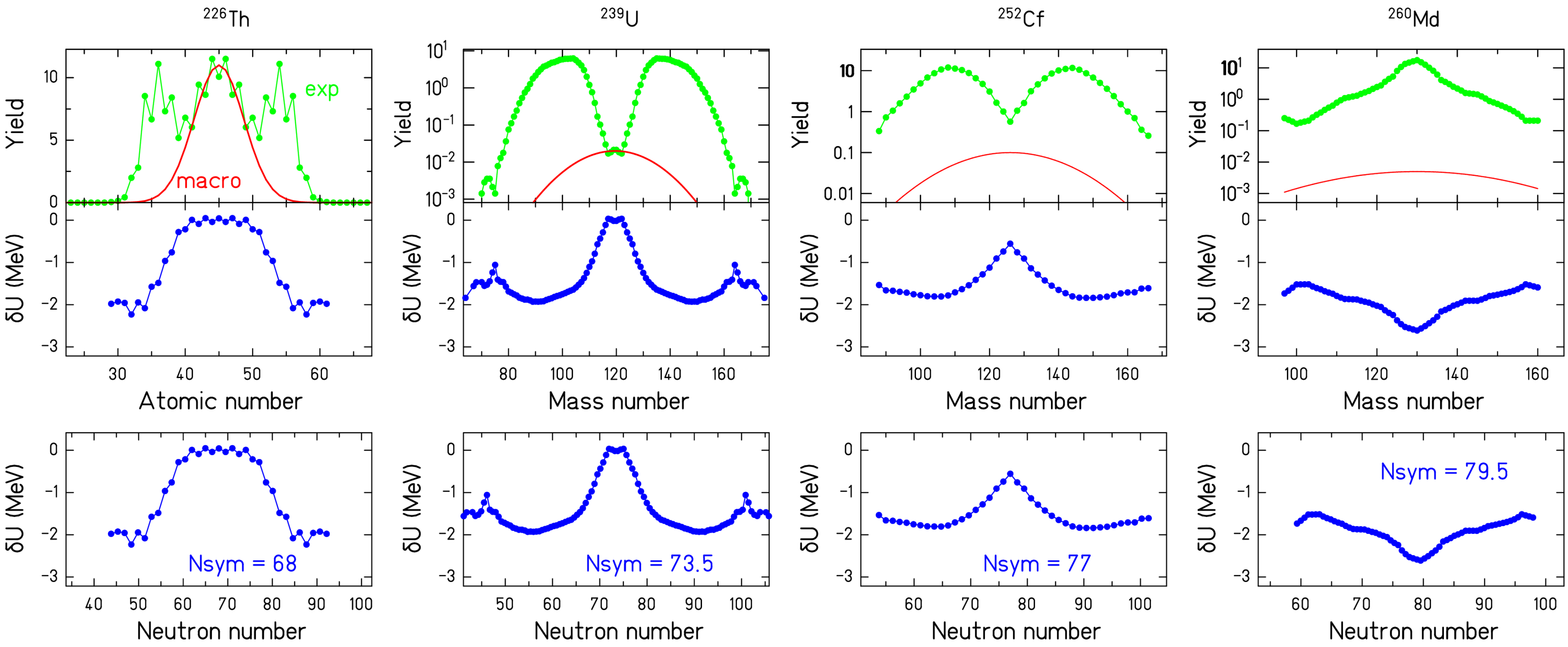
Fission channels:

- Standard 1,
- Standard 2,
- Superasymmetric

Parameters:

- Depth (universal)
- Width (universal)
- Position (systematics, constant in Z, ← see figure)

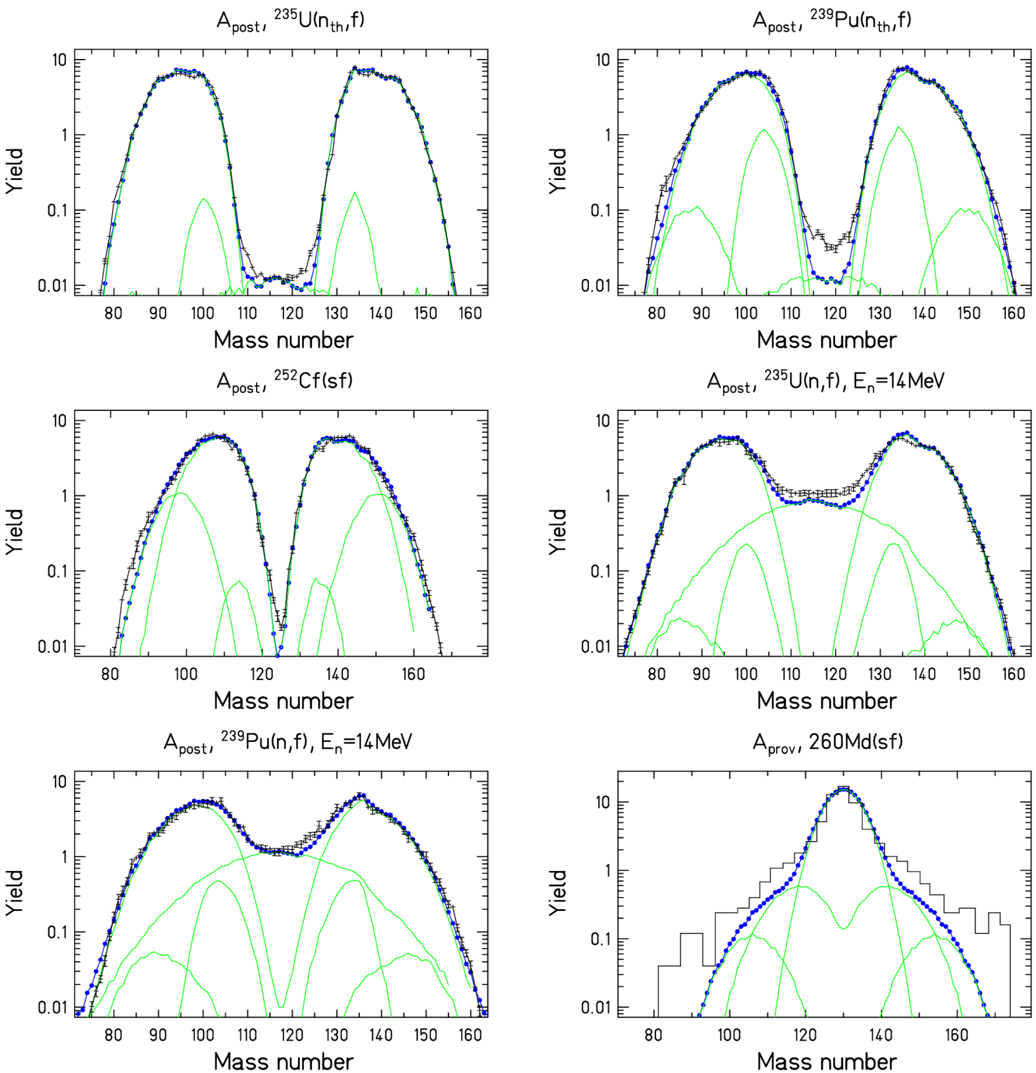
Variation by macroscopic potential



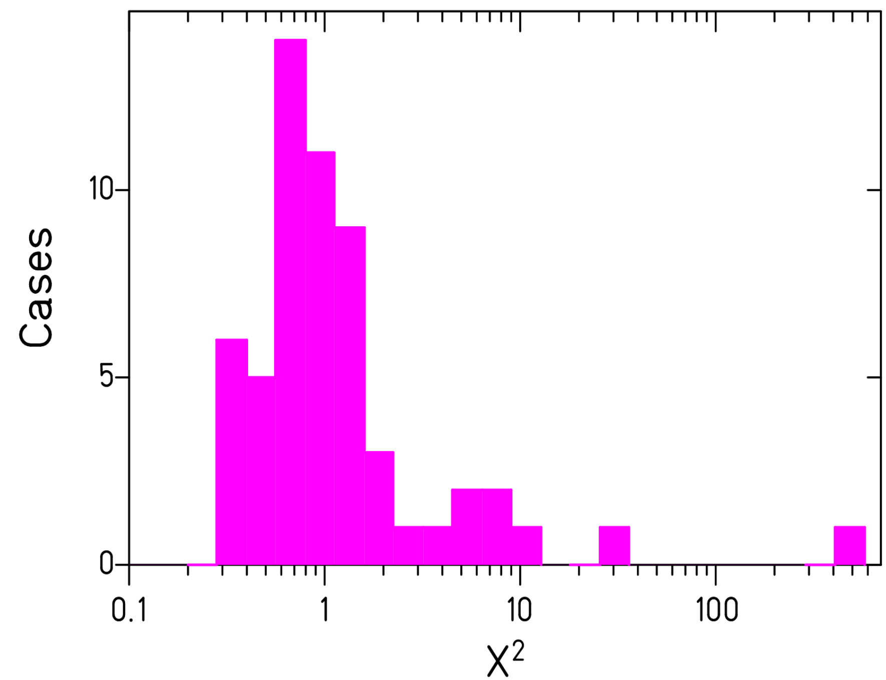
- Symmetric fission channel: Favoured by macroscopic Pot.
- Asymmetric fission channels: Created by shells.

The position of symmetry (in A, N, Z) shifts with respect to the shells of the fission modes.
→ Main reason for changing mass distributions.

Quality of mass yields from GEF



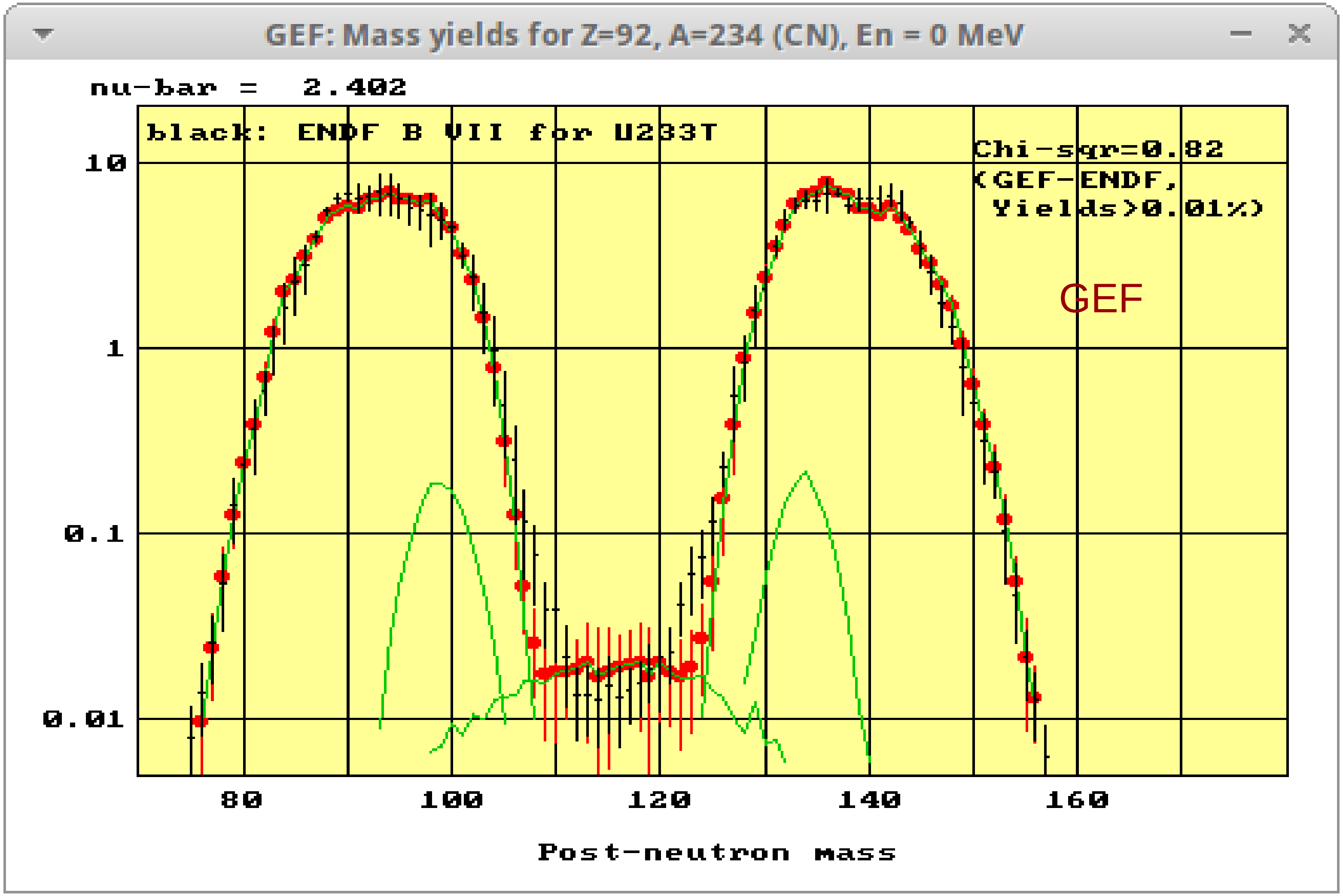
Chi-squared deviations per system



Excerpt from K.-H. Schmidt et al., Nucl. Data Sheets 131 (2016) 107

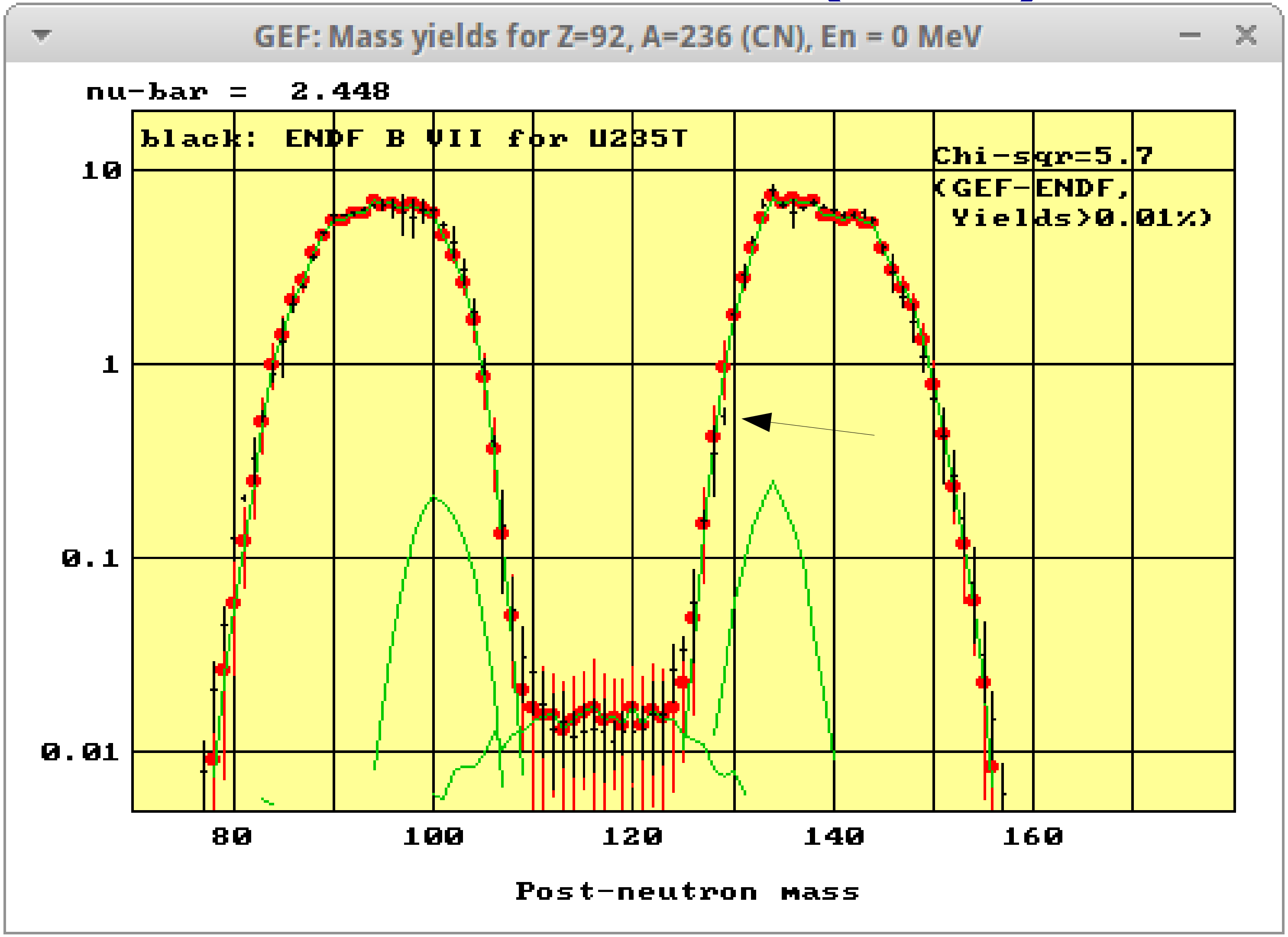
Almost all large deviations caused by erroneous evaluation (evidenced by GEF)!

The “normal” case 233U(nth,f)



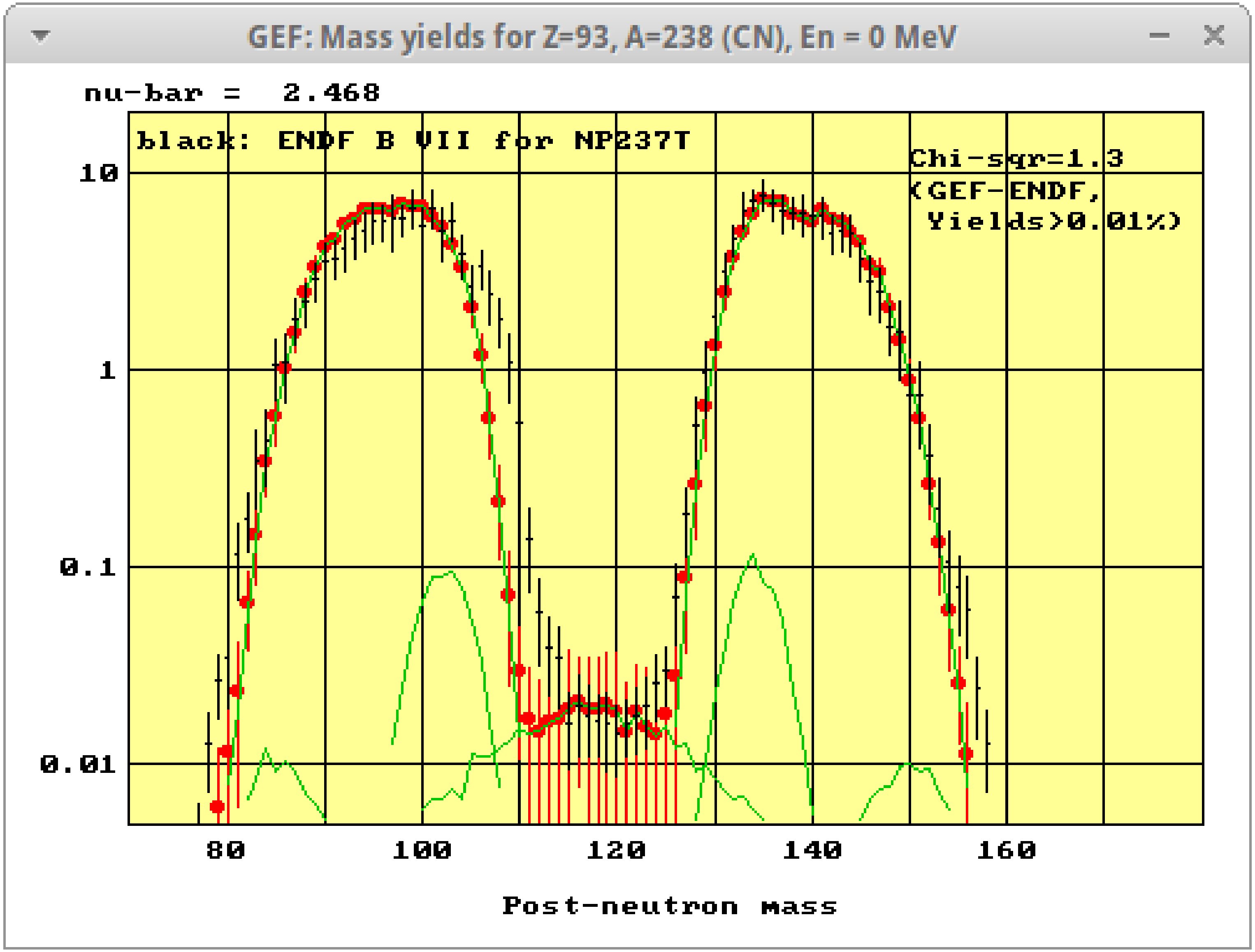
- Chi-squared around 1.
- Most model uncertainties smaller than exp. errors.
- No indication for erroneous data.

The case 235U(nth,f)



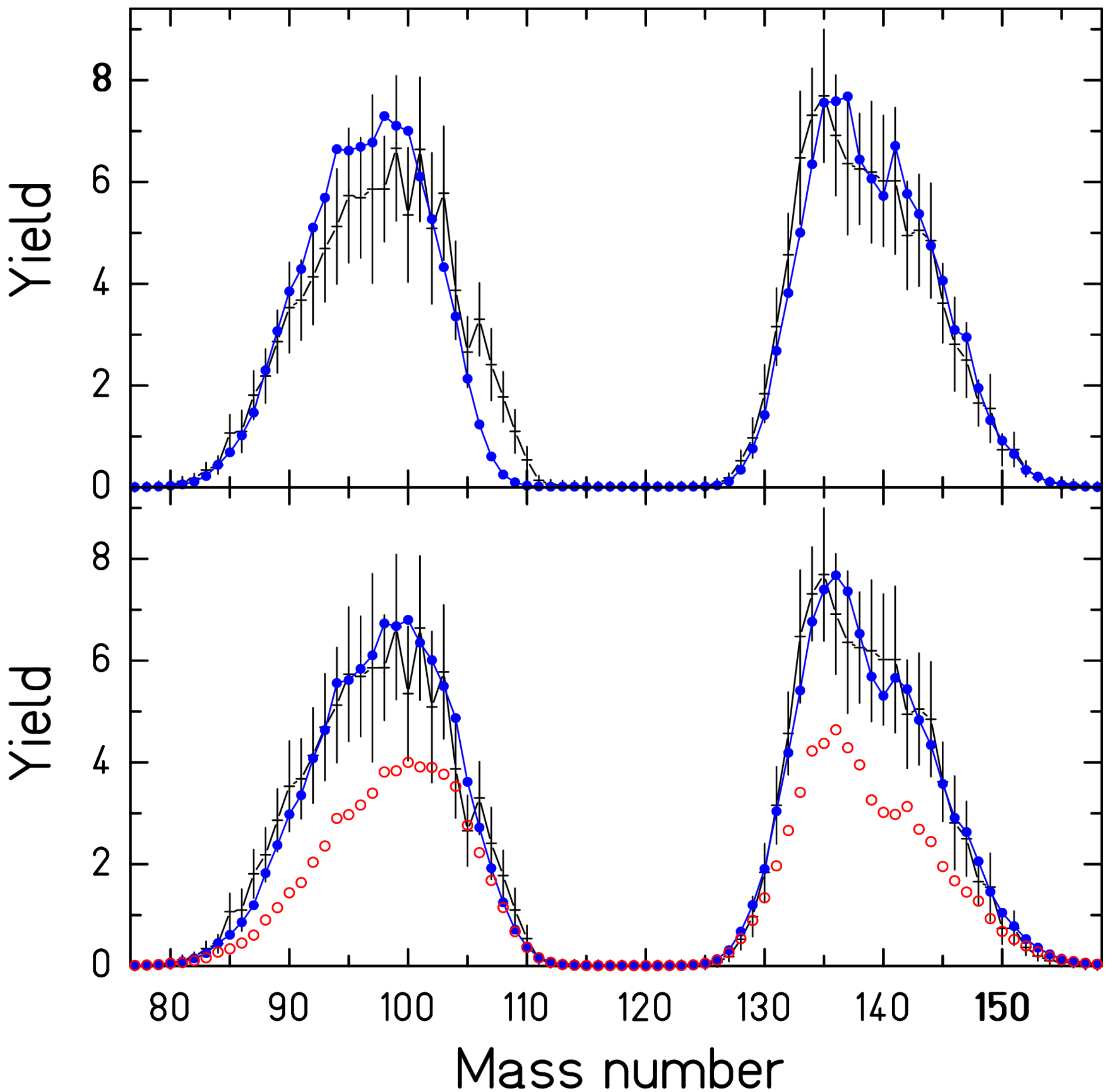
- Many precise experimental data.
- Some model uncertainties are larger than the experimental ones.
- Only few deviations are larger than the exp. error bars
  (experimental problem with Y(A=129)???)

The problematic case 237Np(nth,f)



- Erroneous data due to target contaminant are easily detected (probably 15 ppm 239Pu).

237Np(nth,f), the contributions



Black: Evaluation ENDF/B-VII

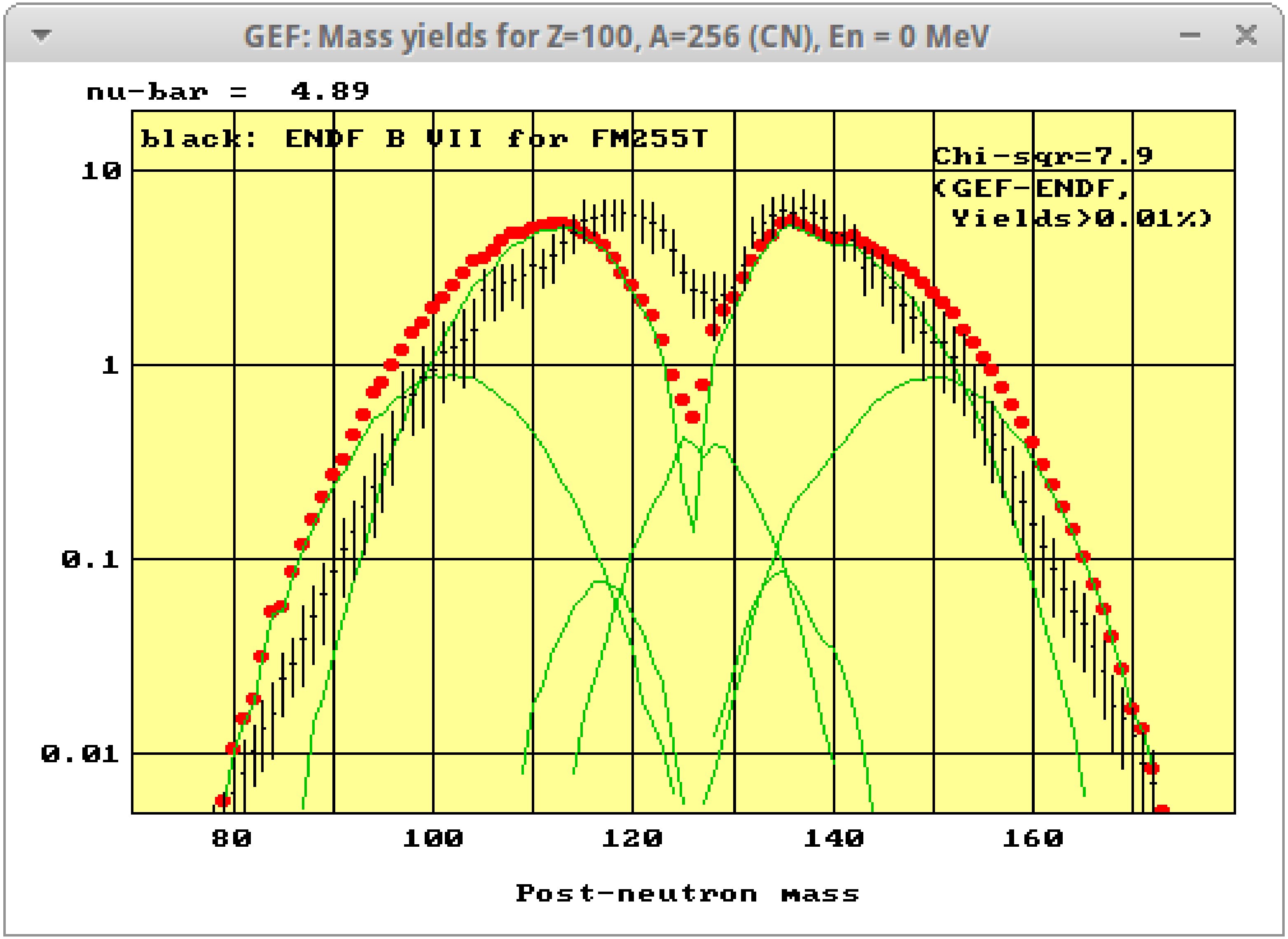
Blue: GEF (pure 237Np)

Blue: GEF (total)

Red:GEF (Contribution from 239Pu)

Also noticeable in the prompt-fission multiplicity.

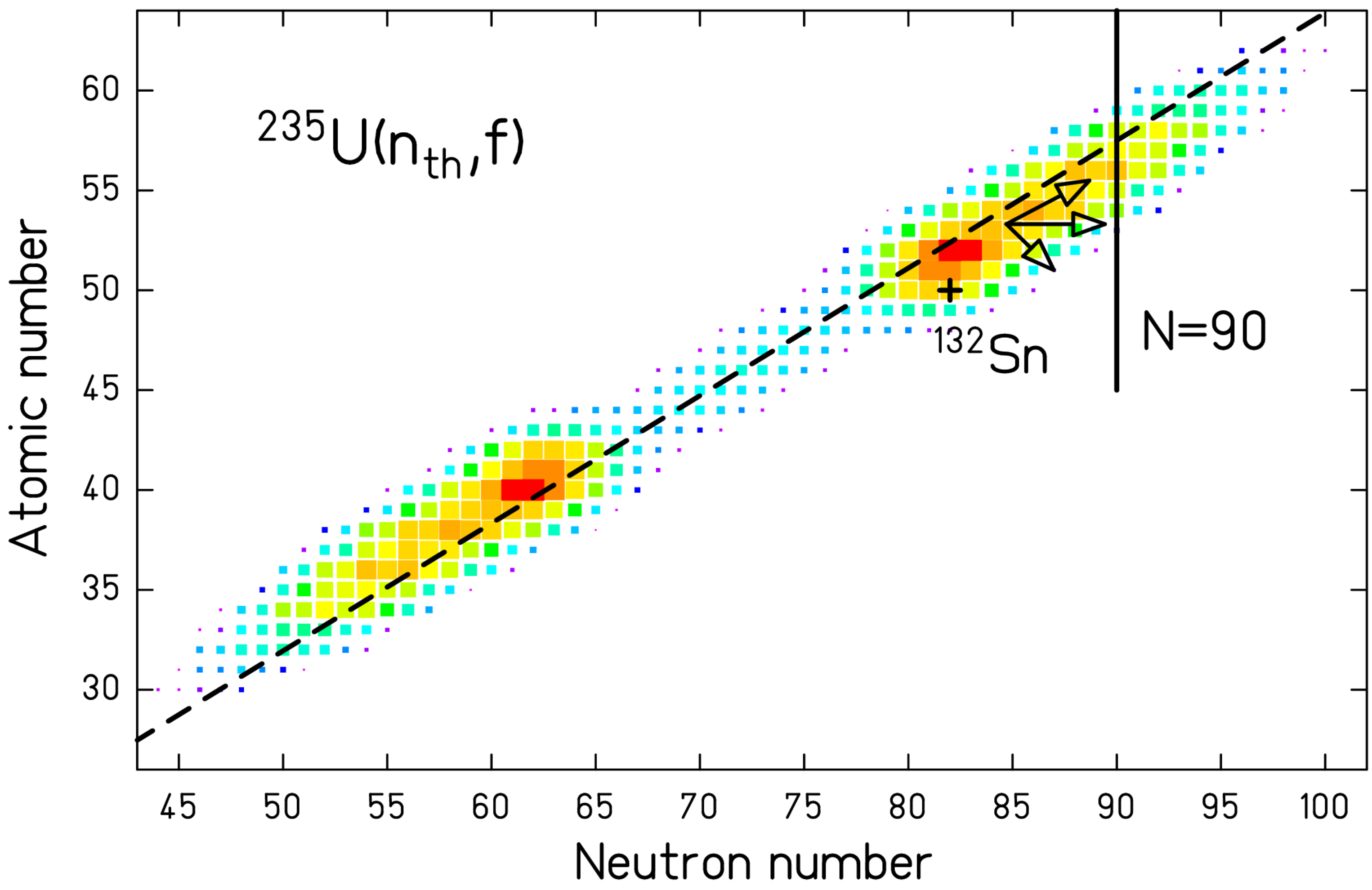
Error in evaluation (ENDF/B-7)



FM255T

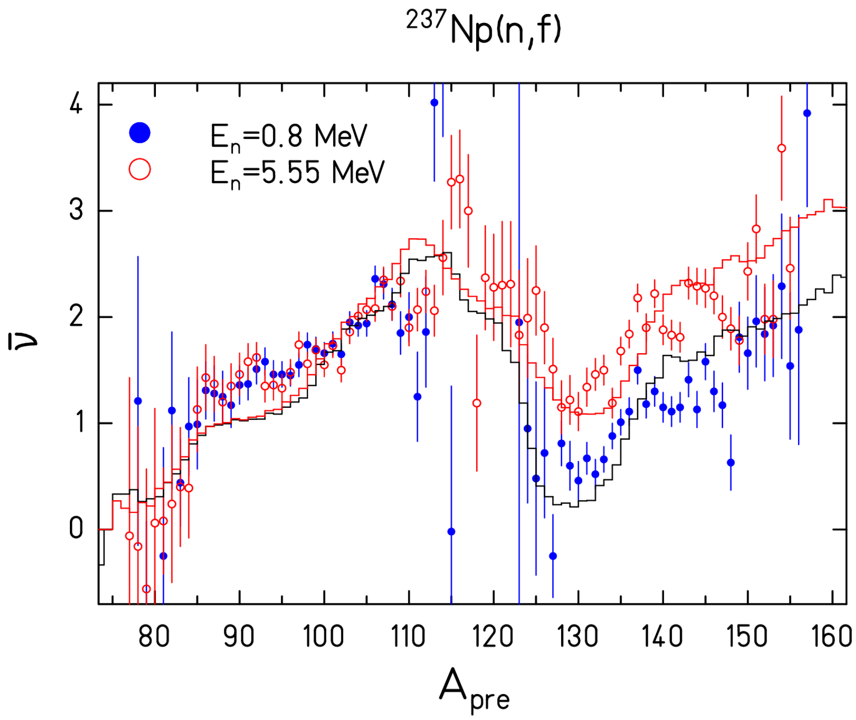
Prompt-neutron multiplicity almost zero:
far from expected value (4.9).

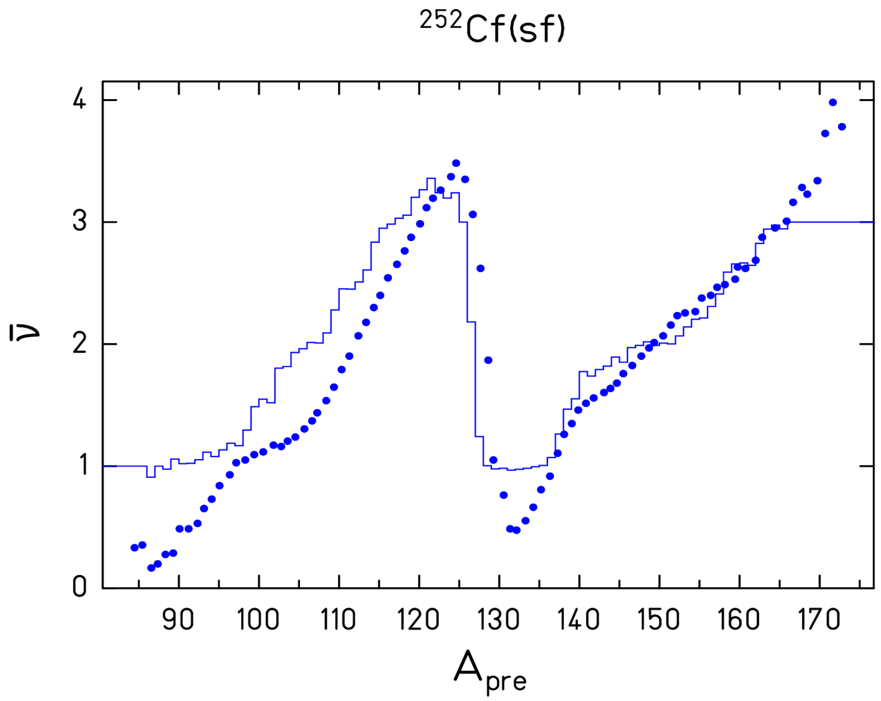
Full nuclide distributions



Pre-neutron: Influence of charge polarization

Prompt neutron emission

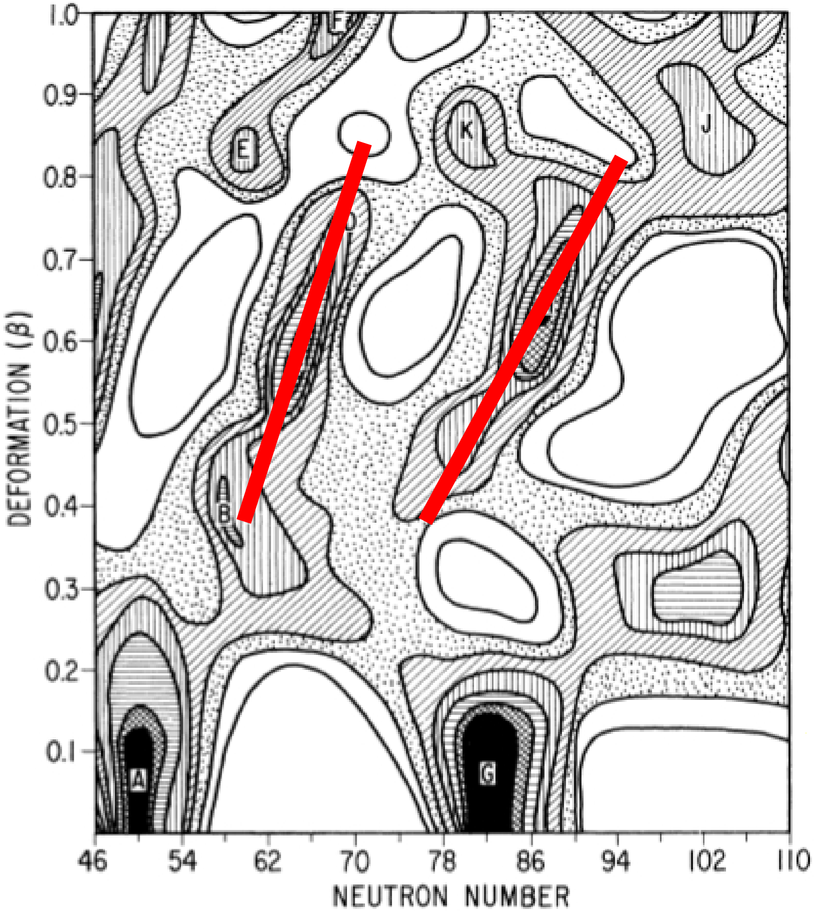




Contributions from different components at scission:

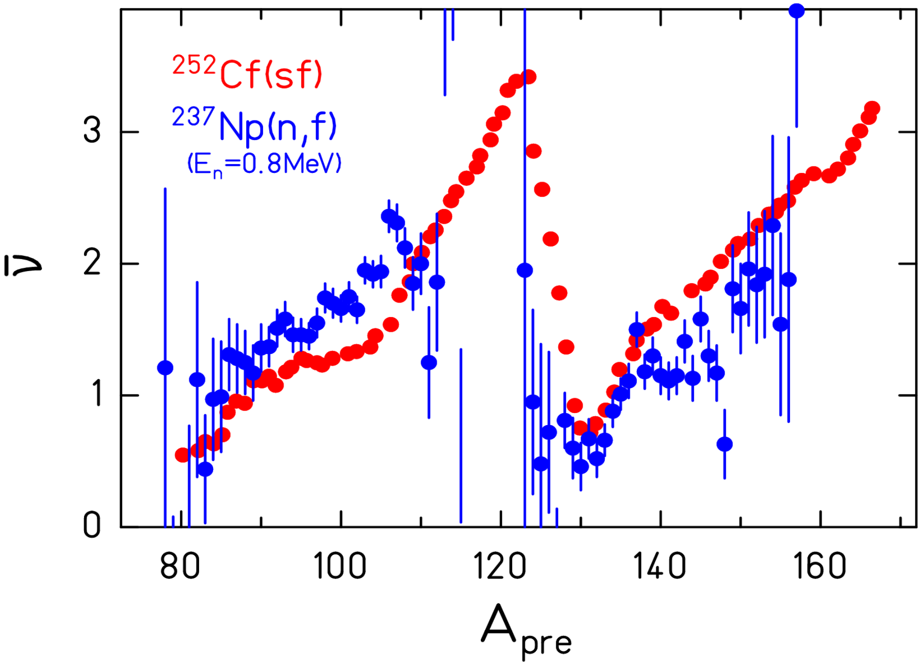
Intrinsic excitation energy (-> energy sorting)
Collective excitations (-> about equal parts)
Deformation (-> structural effects,
responsible for the saw-tooth shape)

Fragment deformation → prompt neutrons



Wilkins et al., Phys. Rev. C 14 (1976) 1832

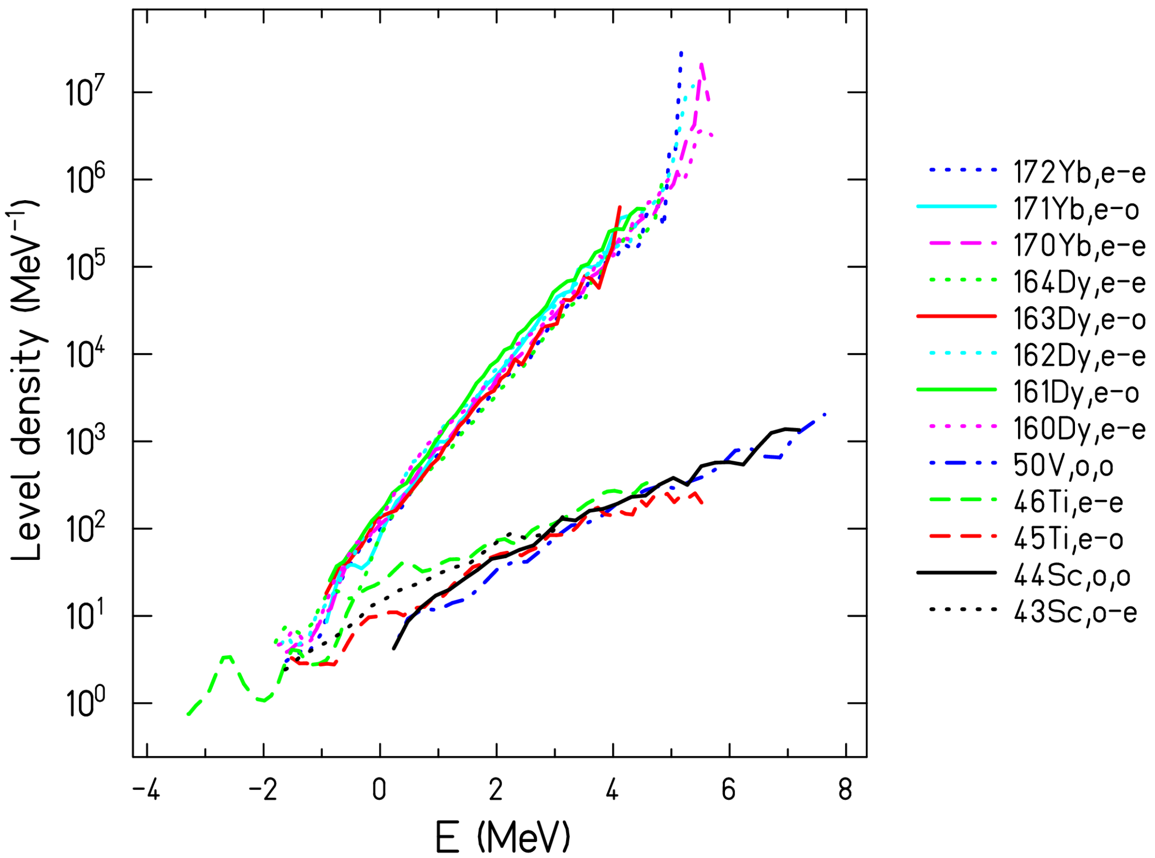
General systematics of deformed shells:
Correlation particle number ↔ deformation
(Additional influence of mac. potential.)

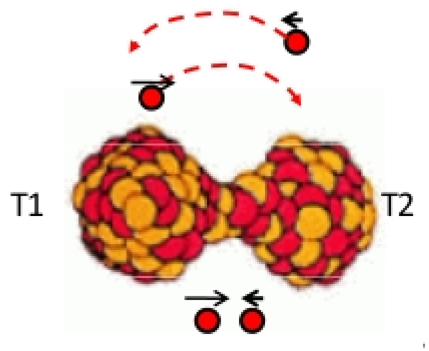


Naqvi et al, 1986 / Zeynalova et al., 2012

Saw-tooth behaviour reflects fragment deformation at scission.

New results on level densities suggests energy sorting in fission





Nascent fragments:

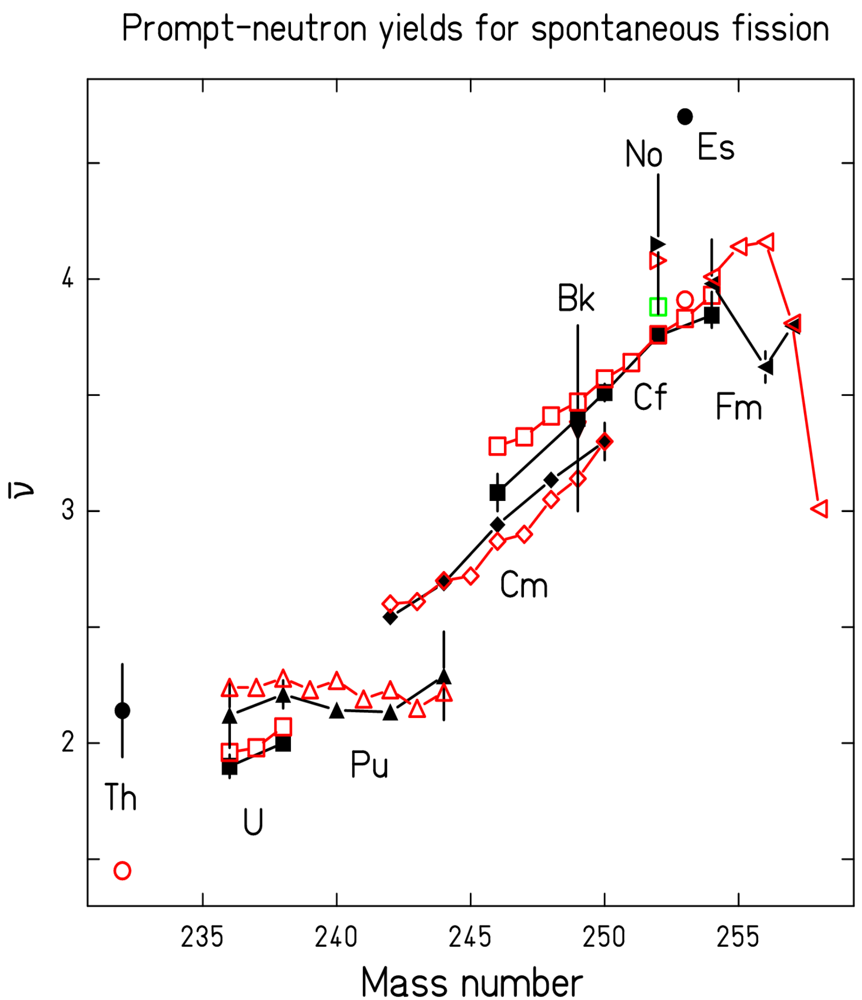
Two thermostats in contact.
→ Energy sorting

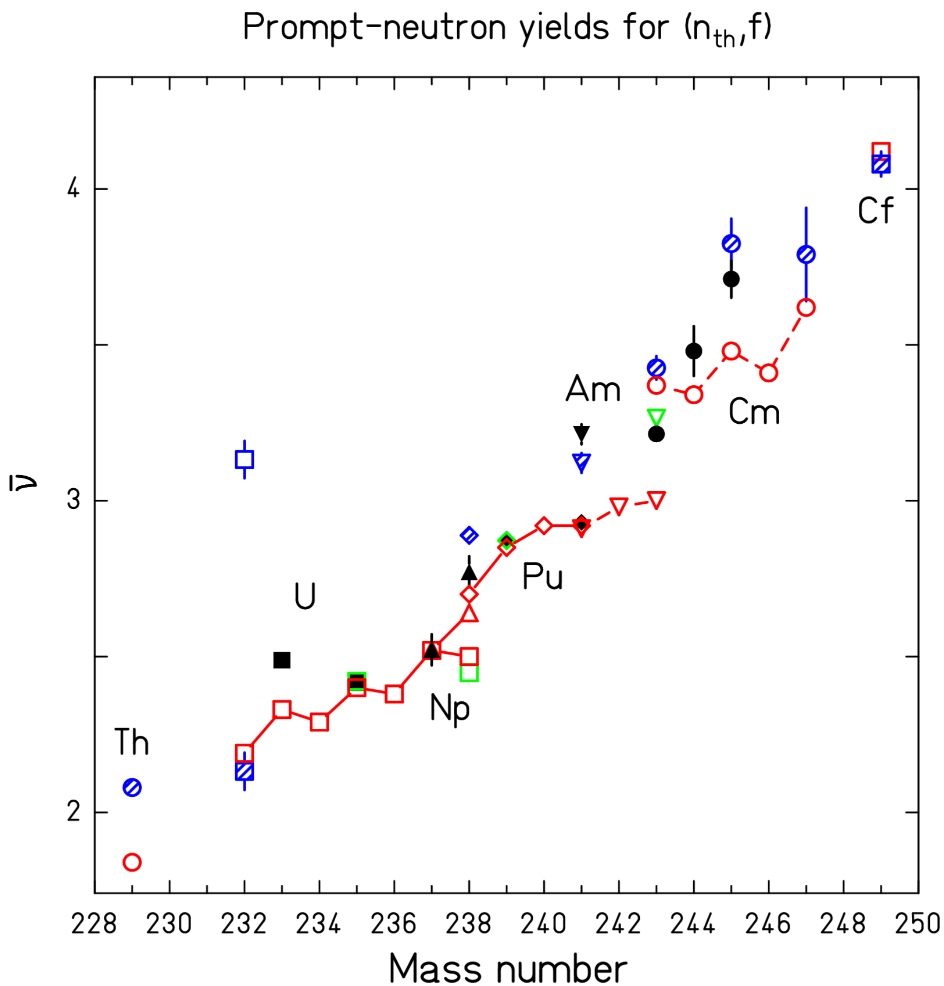
Guttormsen et al. 2012

Schmidt, Jurado,
PRL 104 (2010) 212501

Constant nuclear temperature at low E*.

nu-bar



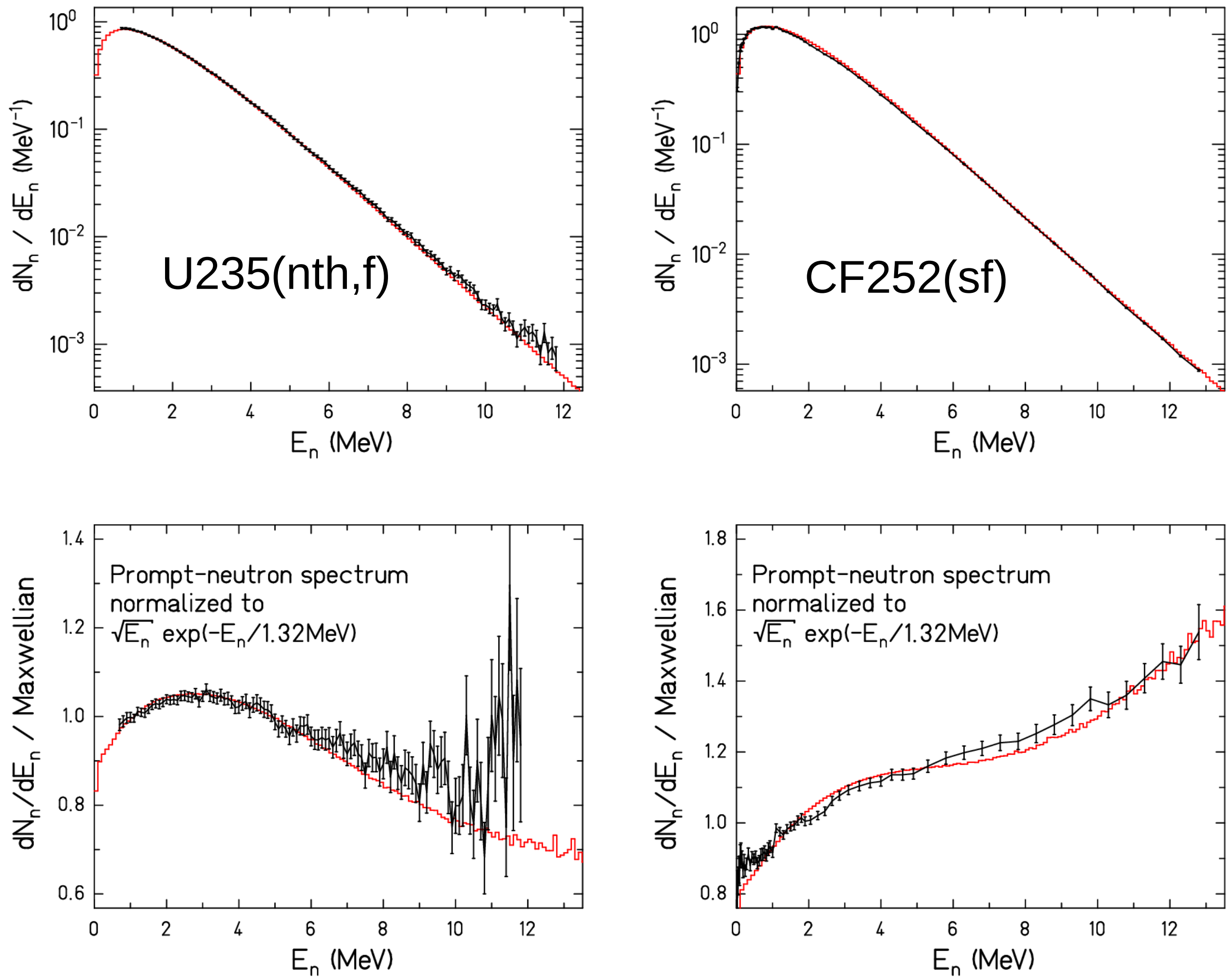


rms deviation: 0.1 units

rms deviation: 0.2 units

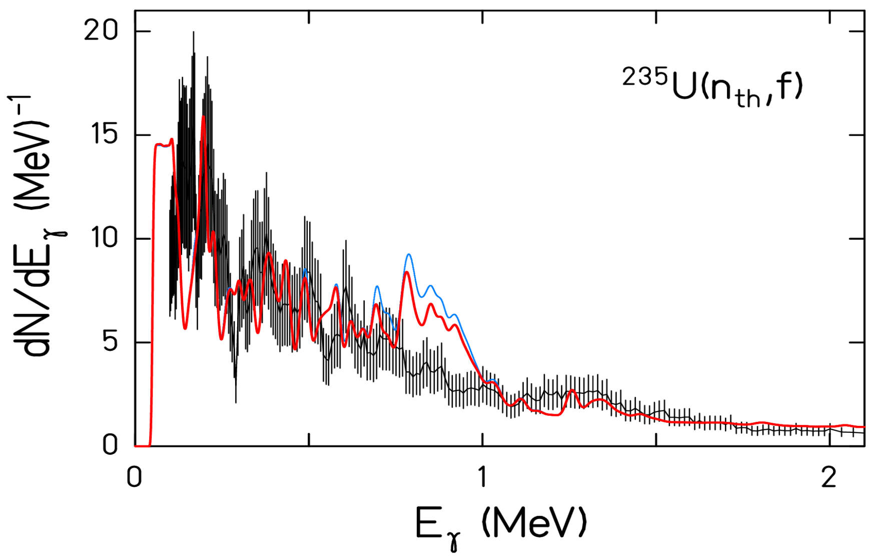
(experimental problems?)

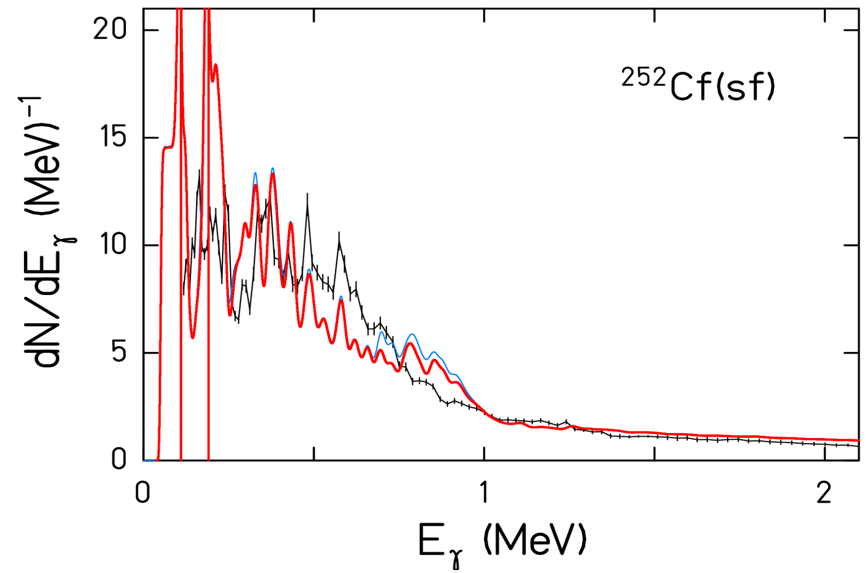
Energy spectra of prompt neutrons

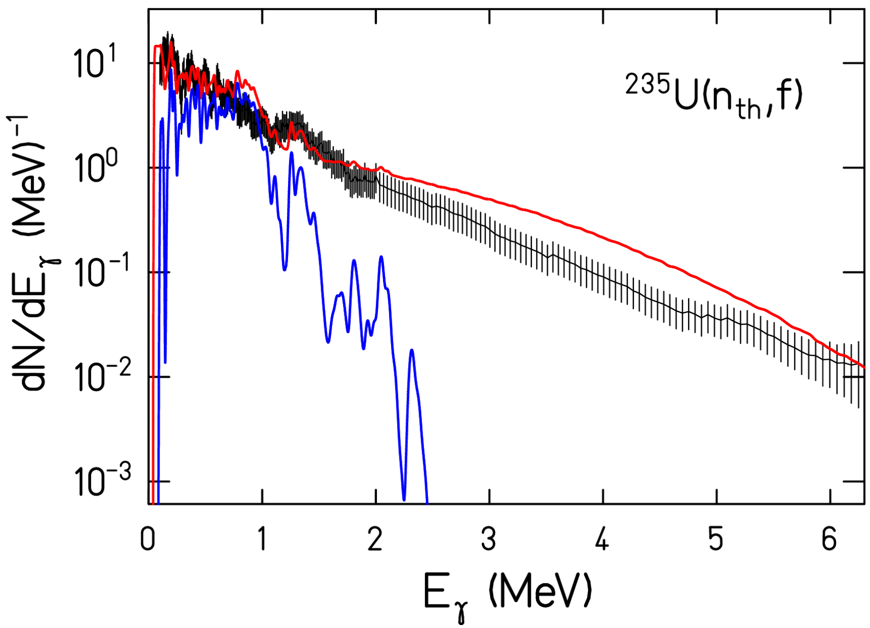


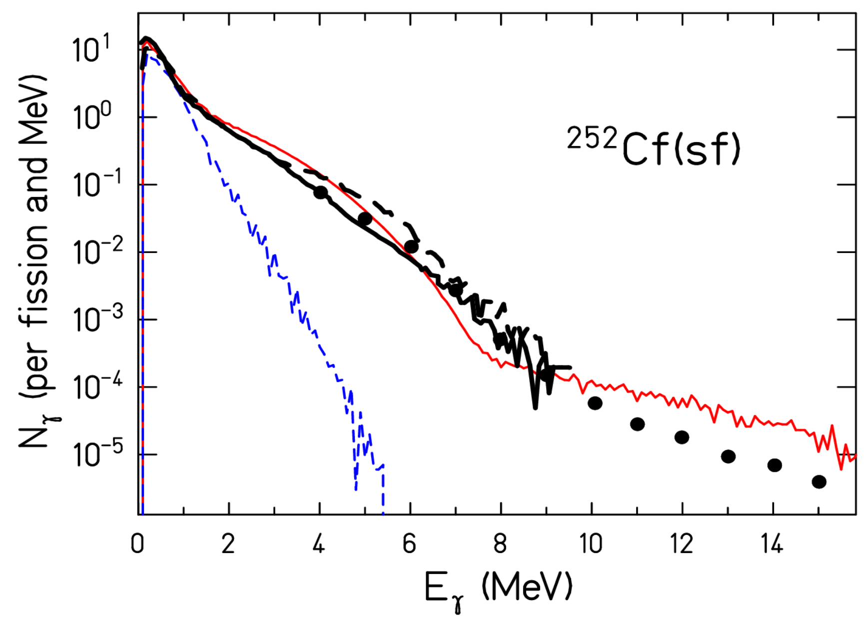
Clue: Modified composite Gilbert-Cameron nuclear level density.
(Increased condensation energy, collective enhancement)
K.-H. Schmidt, B. Jurado, Phys. Rev. C 86 (2012) 044322

Energy spectra of prompt gammas

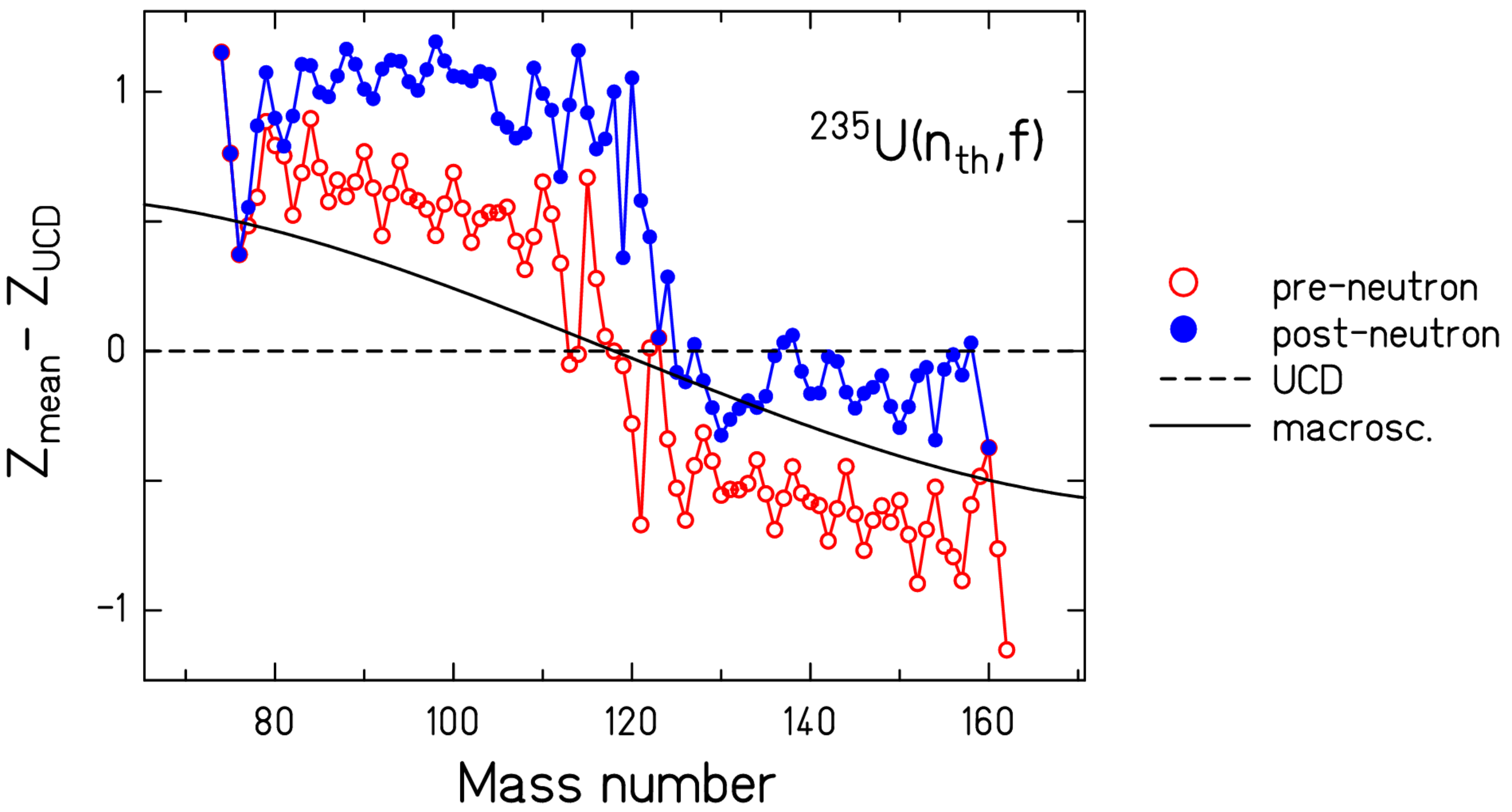




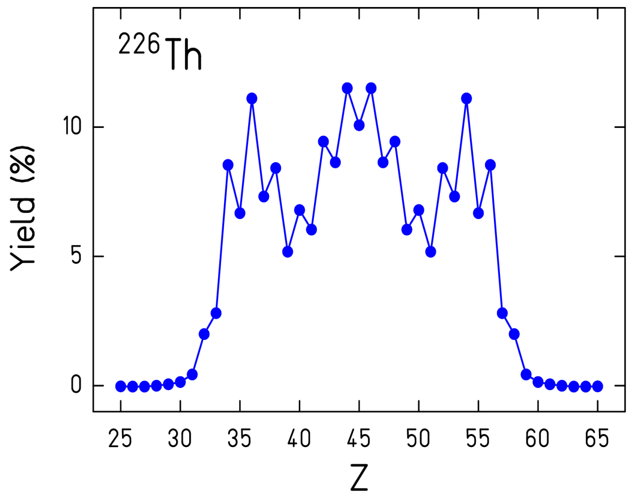




Influence of neutron emission

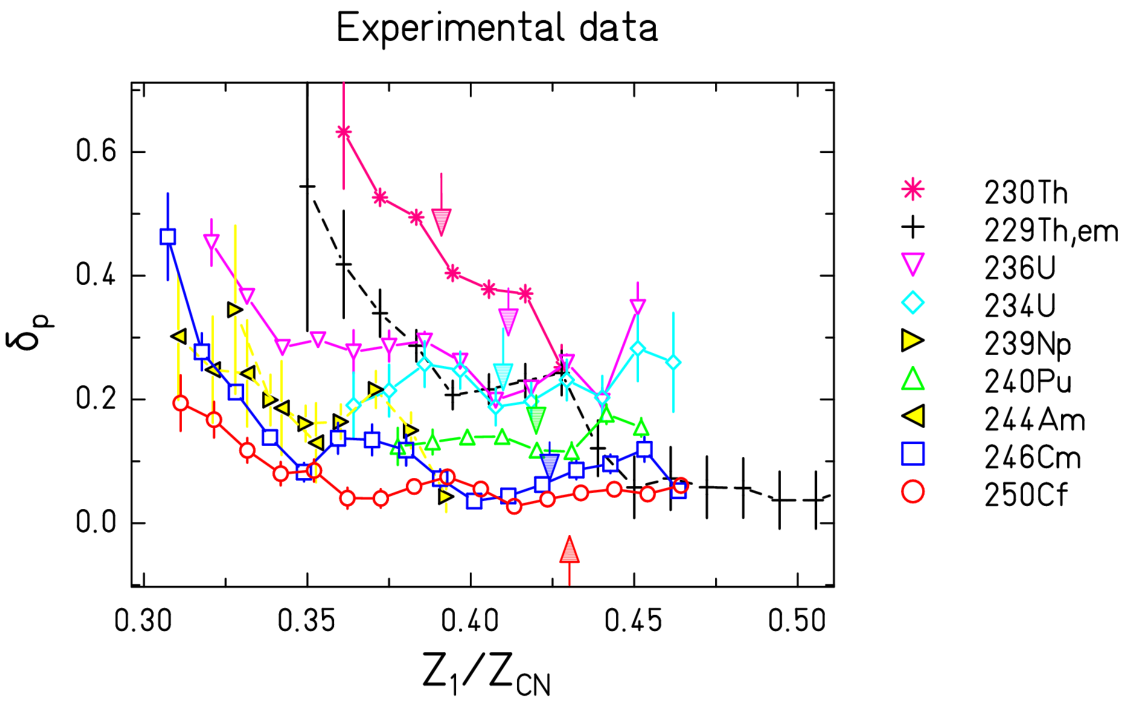


Influence of asymmetry on even-odd effect



K.-H. Schmidt et al.,
Nucl. Phys. A 665 (2000) 221

GSI-experiment:
Z distribution measured over the whole range.

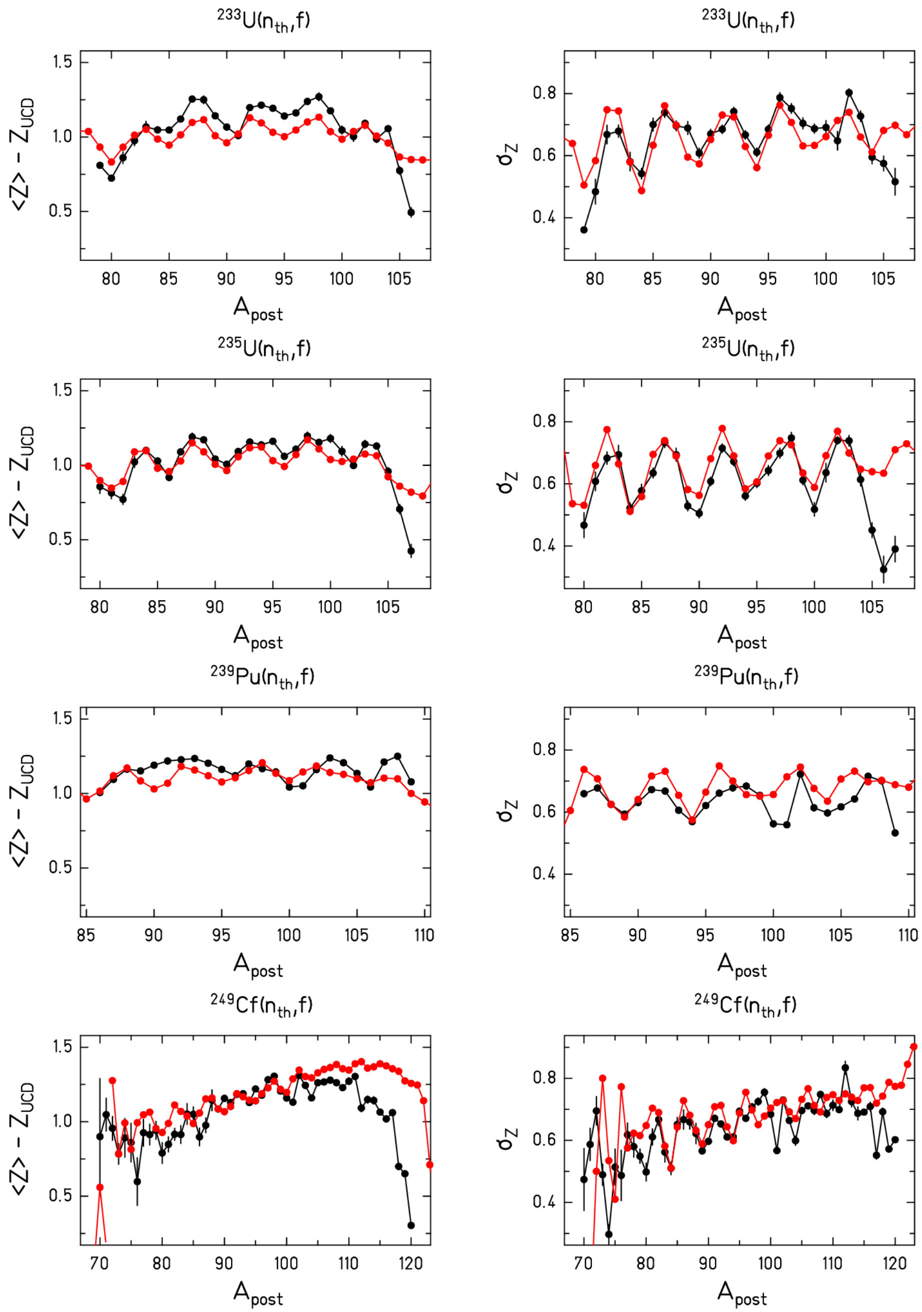


Caamano et al., JPG 38 (2011) 035101

Systematics:
Even-odd effect strongly enhanced in asymmetric splits.
→ **even-even light fragments = end products of energy sorting**

B. Jurado, K.-H. Schmidt, J. Phys. G: Nucl. Part. Phys. 42 (2015) 055101

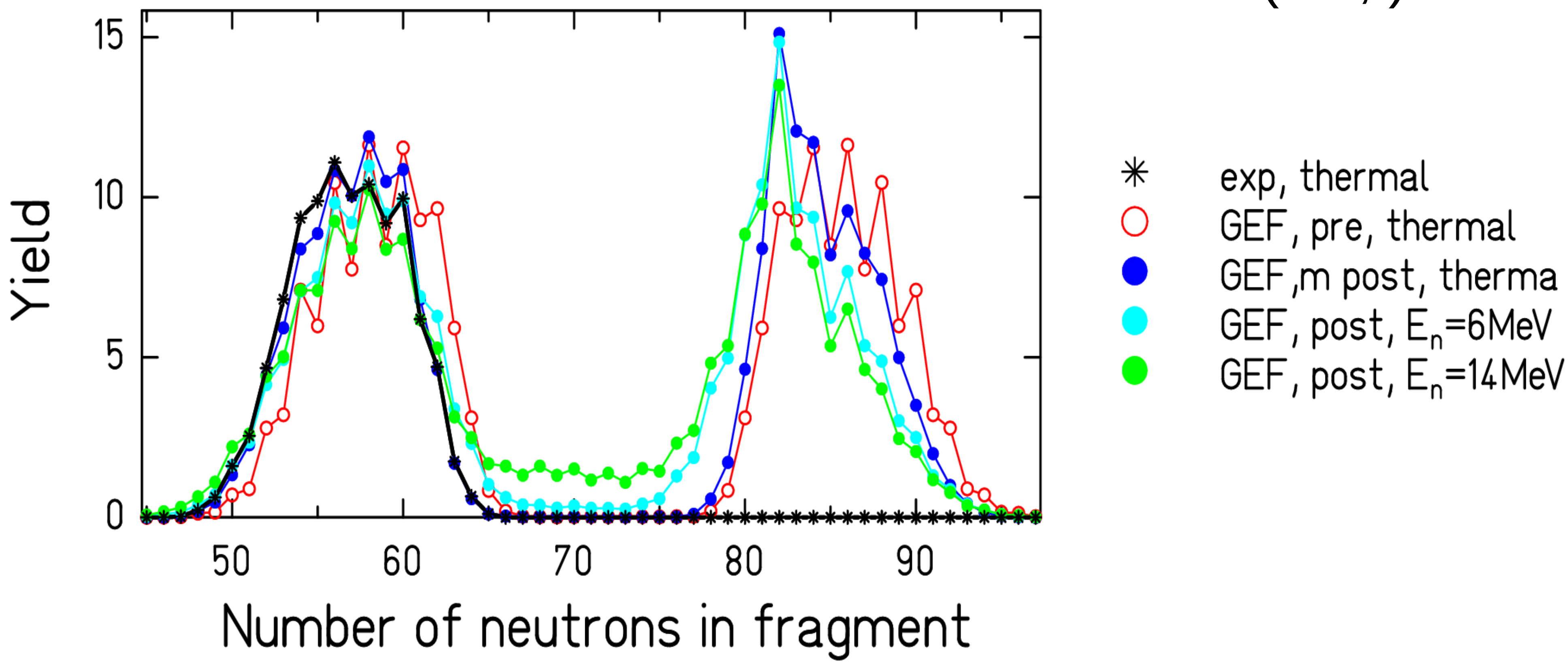
Isobaric sequences



Influence of charge polarization at scission and prompt-neutron emission.

Even-odd effect in ff neutron number

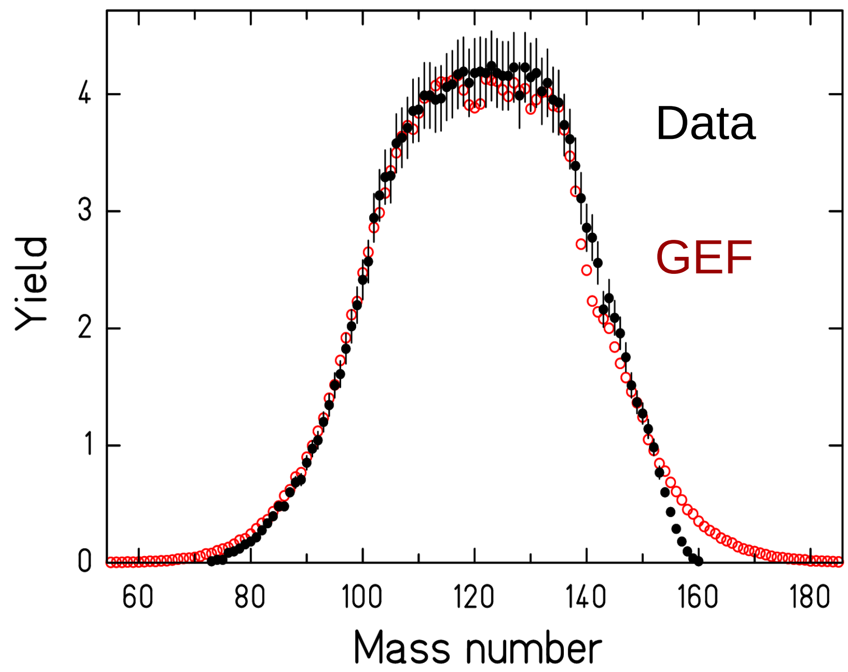
235U(nth,f)

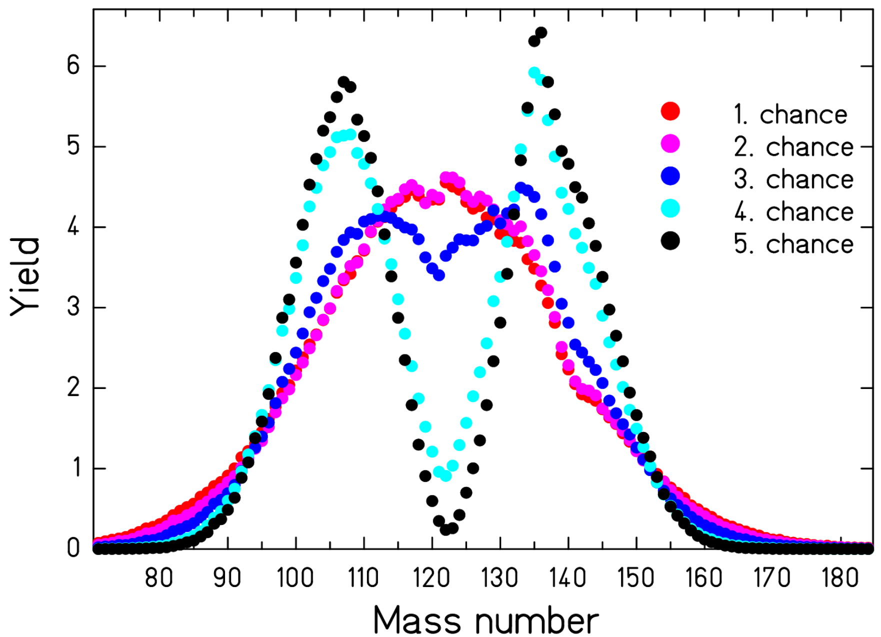


Even-odd effect in neutron number of fragments (post-neutron) is created by evaporation. (Does not depend on E*!)

By influence of pairing on binding energies and level densities:
M. V. Ricciardi et al., Nucl. Phys. A 733 (2004) 299

Multi-chance fission





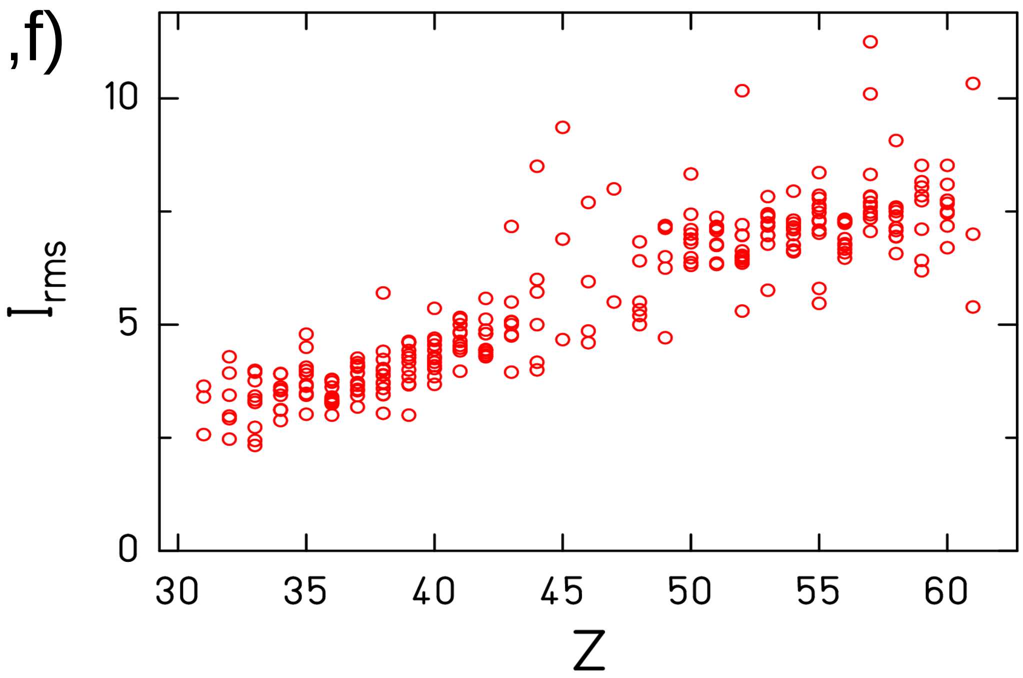
250Cf, E* = 45 MeV
VAMOS experiment

GEF: Contribution of fission chances

GEF: The final FF distribution is the sum of the different fission chances.

Fragment angular momentum

235U(nth,f)



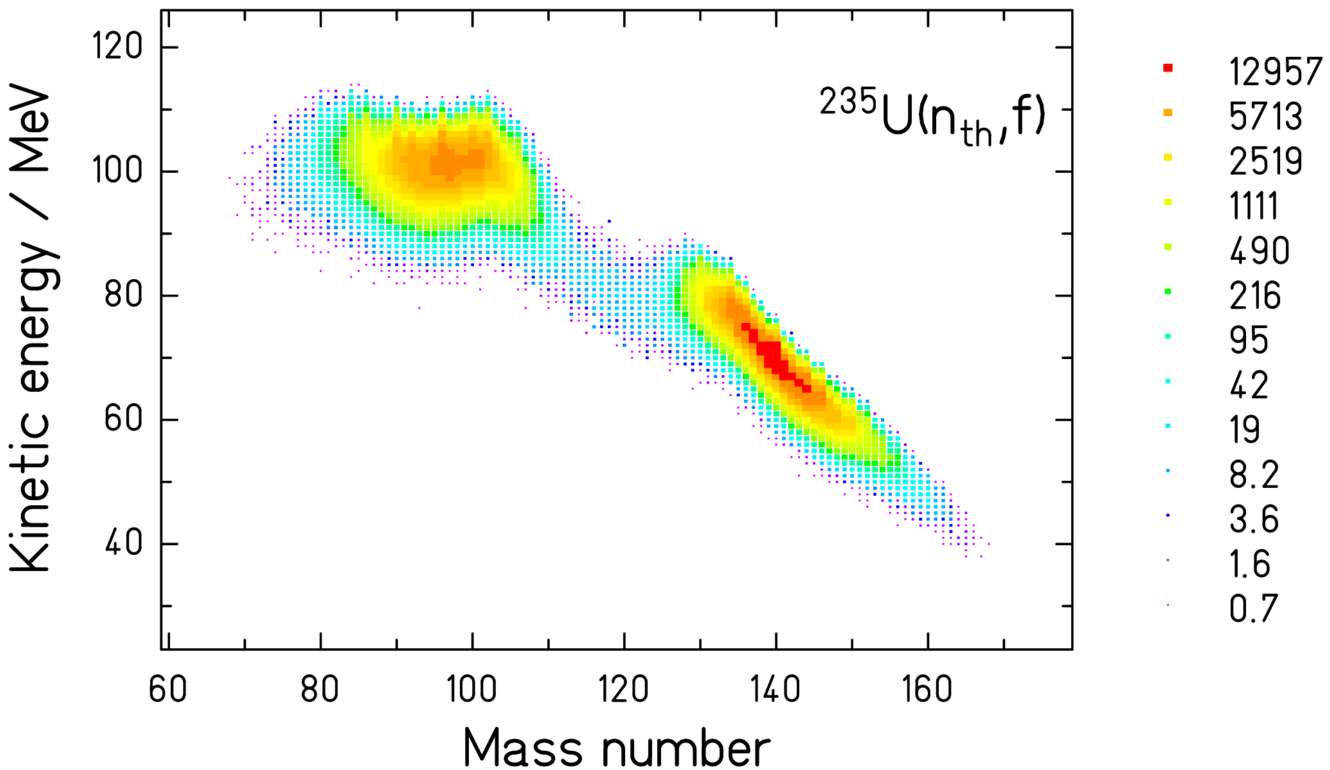
GEF calculations

in good agreement with measured isomeric ratios

Theory: “Pumping” from q.m. uncertainty of orbital angular momentum (Kadmensky) + l of unpaired nucleons.

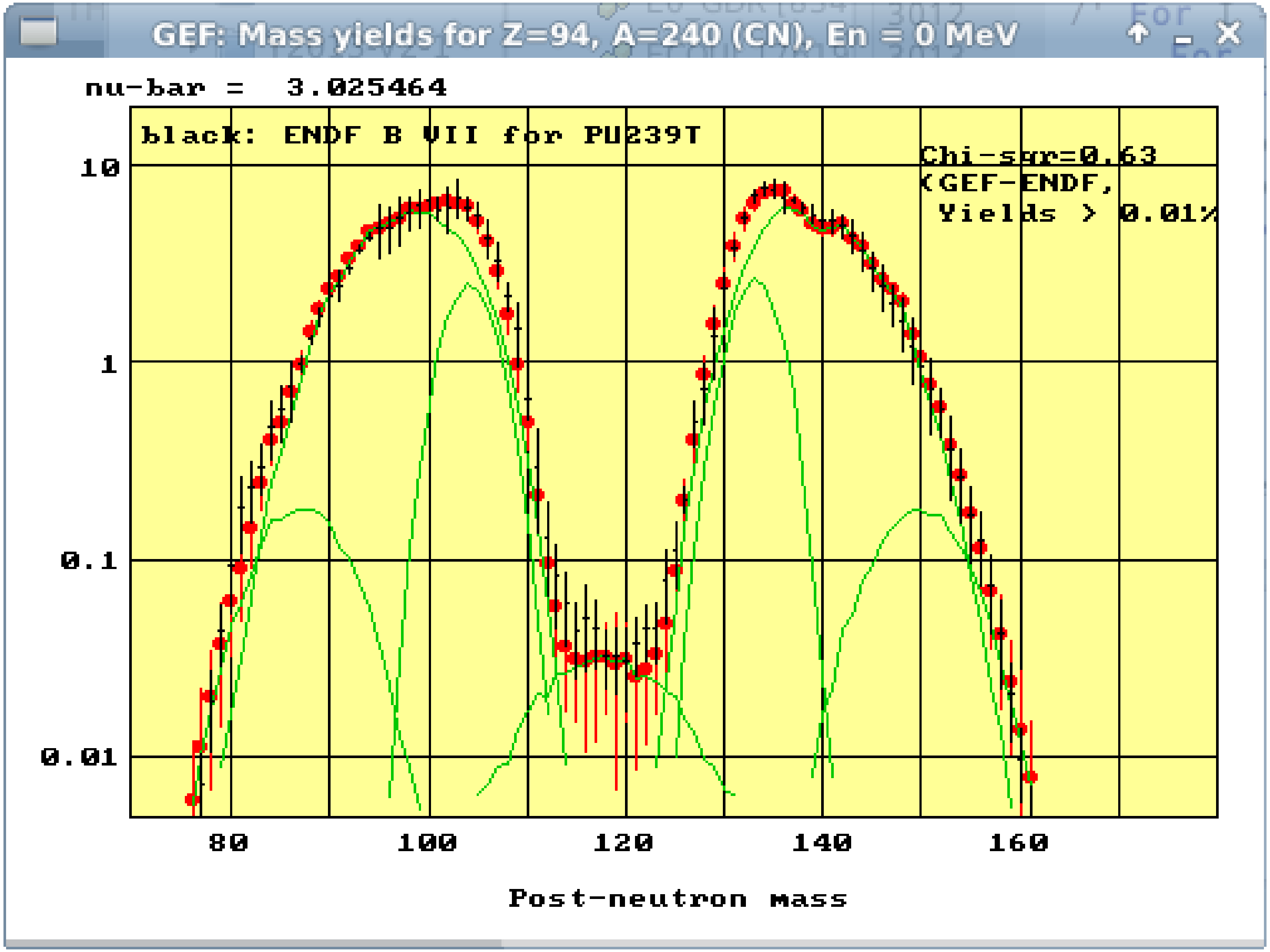
Fragment angular momentum
- stores collective energy at scission (less TKE)
- feeds contributions of rotational transitions to prompt gamma spectrum

GEF: A - TKE



$^{235}U(n_{th},f)$
Kinetic energy / MeV
Mass number
120
100
80
60
40
60
80
100
120
140
160
12957
5713
2519
1111
490
216
95
42
19
8.2
3.6
1.6
0.7

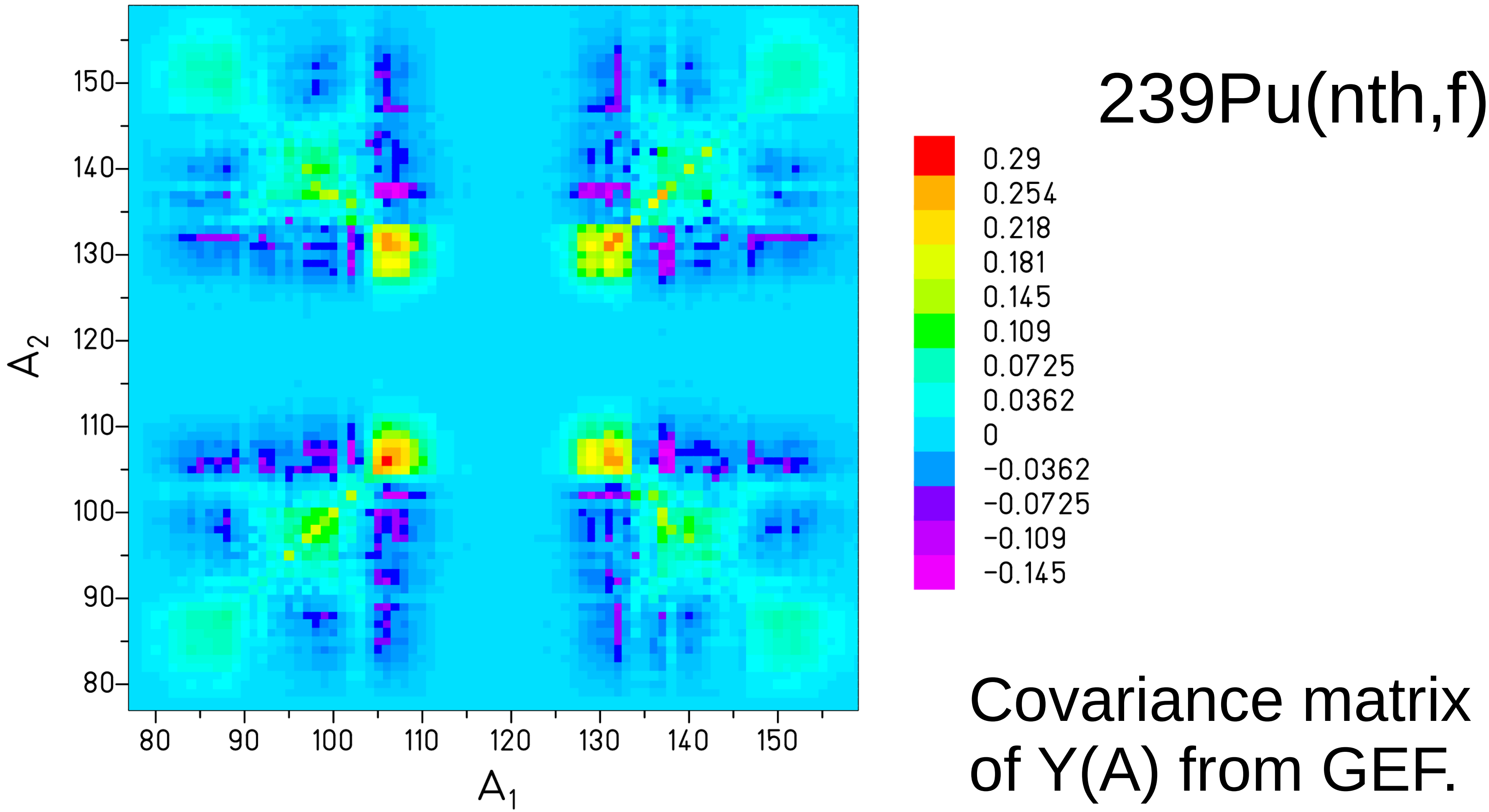
Uncertainties of the model



Mass yields from GEF with estimated uncertainties.

GEF calculations with perturbed parameters.

Covariances from GEF



Covariance matrix of Y(A) from GEF.

Correlations or covariances available for any pair of fission observables or between the fission quantities of different systems

Summary

- GEF: Description of the fission process on an “intermediate” level with a rigid theoretical frame and empirical parameters.
- High precision, good predictive power over a large range of nuclei.
- Fast code (10^6 events in ≈ 1 minute).
- Freely available, open source.
- Suited to detect erroneous data (validation).
- Covariances, ENDF tables of FY, random files provided.
- See more complete presentation of the GEF code in: "General description of fission observables: GEF model code", K.-H. Schmidt, B. Jurado, C. Amouroux, C. Schmitt, Nucl. Data Sheets 131 (2016) 107.