A new evaluation method based on covariances from the GEF model

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“Improved Fission product yield evaluation methodologies”
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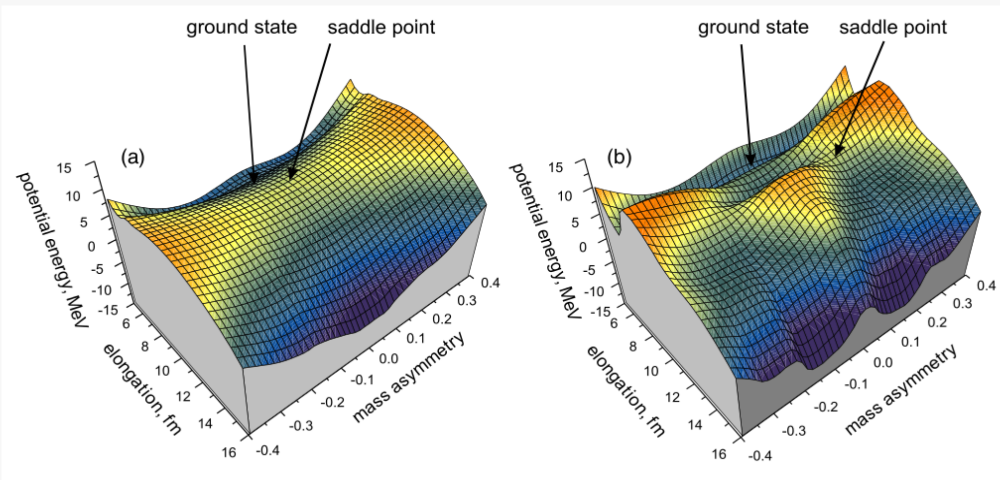
The GEF model

Concept

Potential-energy surface of 238U (Karpov 2008)



Macroscopic properties attributed to CN (empirical from high-energy fission data)

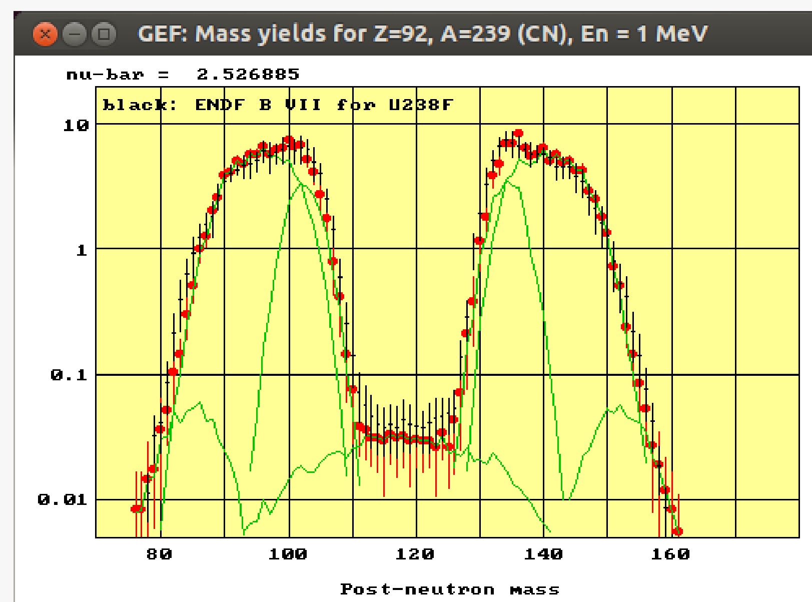
Microscopic properties attributed to fragment shells (empirical from low-energy fission data)

Fission channels
Statistical model at “dynamical freeze-out”
Statistical mechanics → energy sorting
Emission of prompt neutrons and gammas
About 30 specifically adjusted parameters

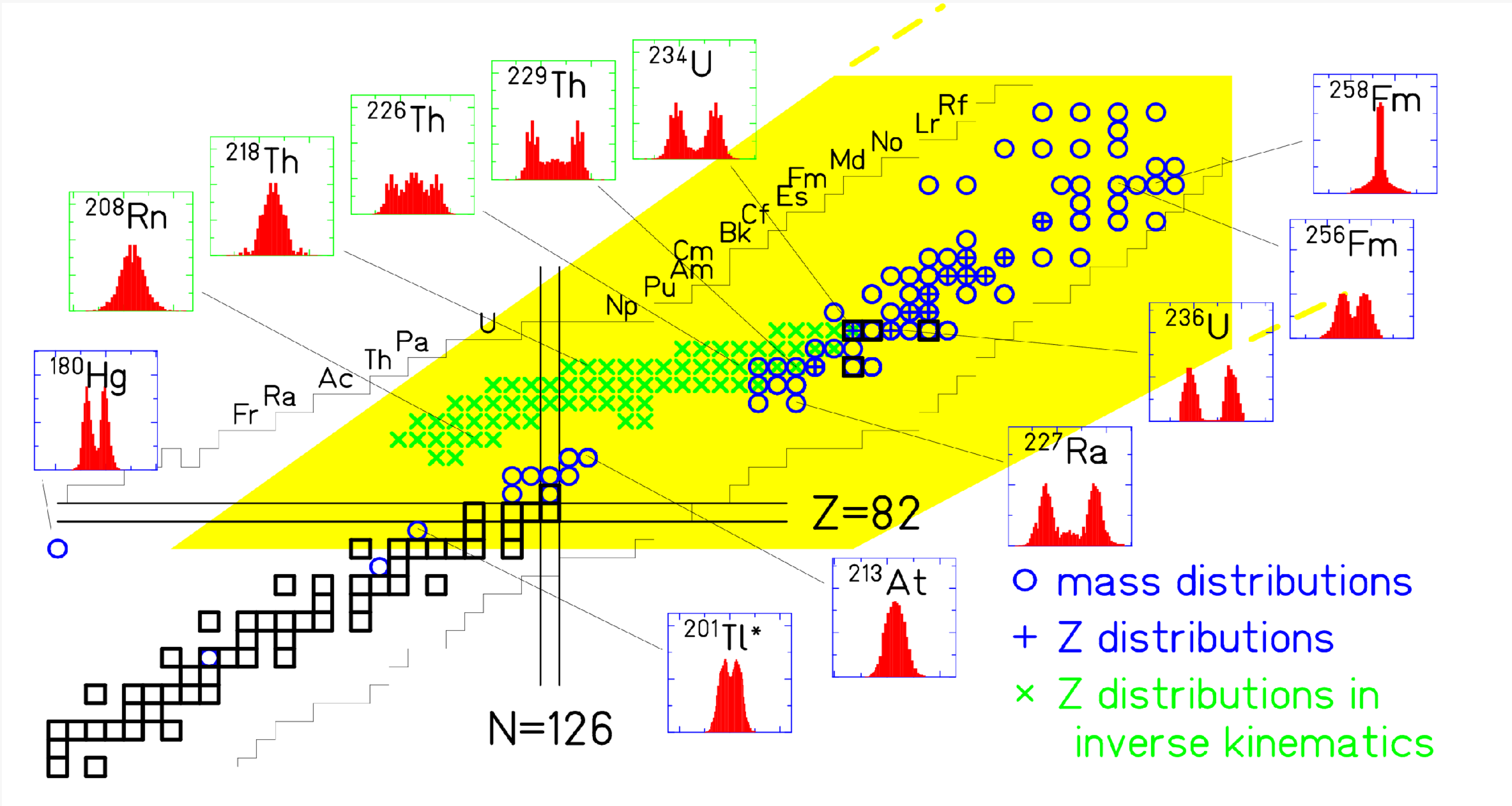
Results

Monte-Carlo code calculates for each fission event:

A1,A2 pre/post-neutron
Z1,N1,Z2,N2 pre/post-neutron
TKE pre/post-neutron
I1,I2 (fragment spins)
nu1,nu2 (# of prompt neutrons)
Ekin of prompt neutrons
# of prompt gammas
E of prompt gammas



Coverage of GEF (marked in yellow)

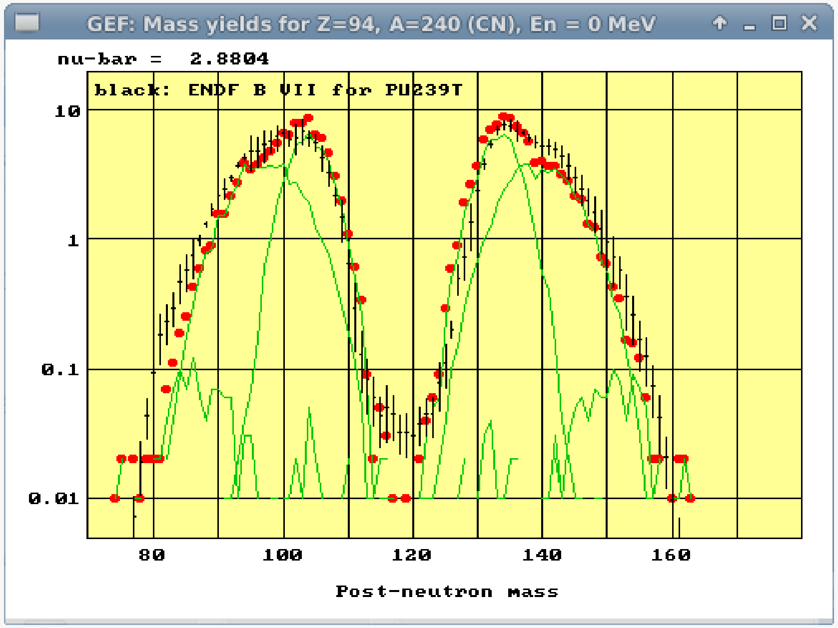


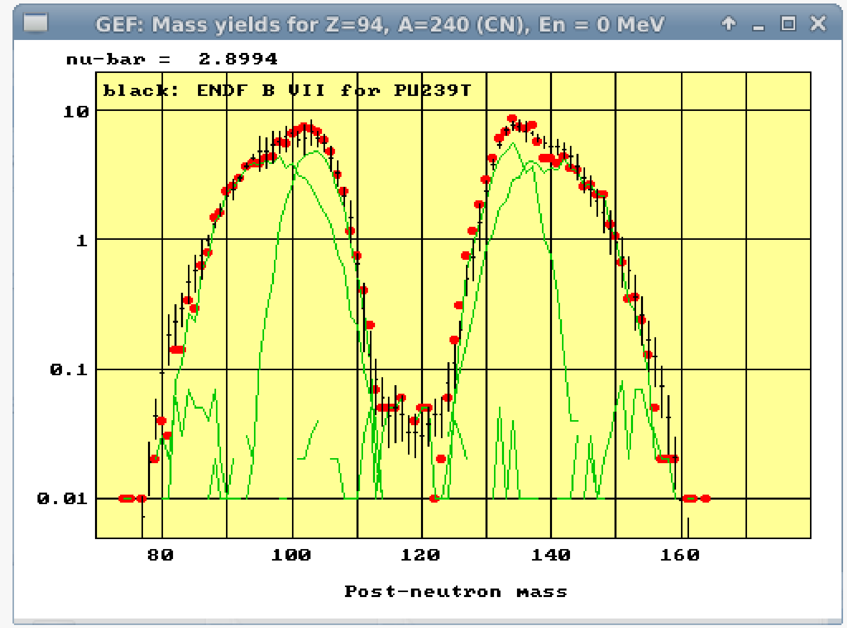
The same parameter set is used for all nuclei.

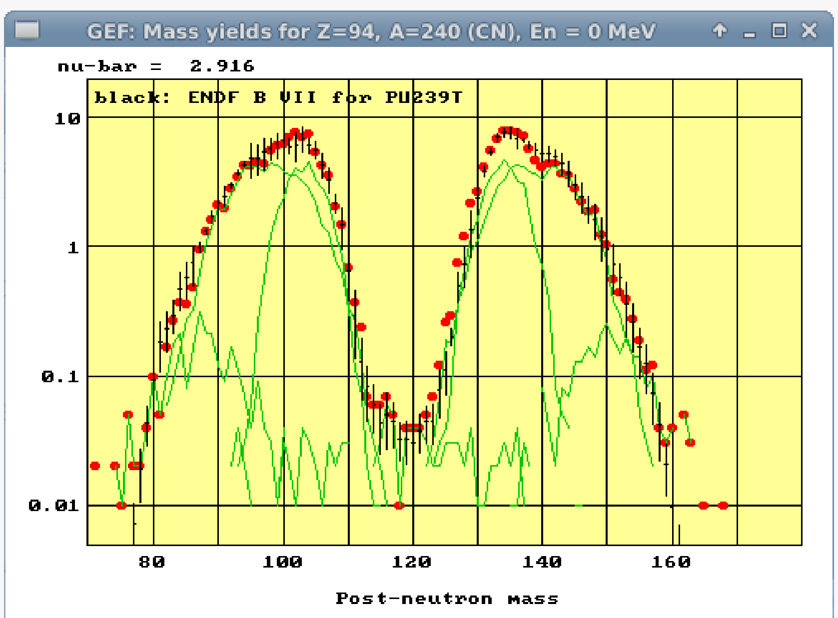
(sf), (n,f) up to En = 20 MeV

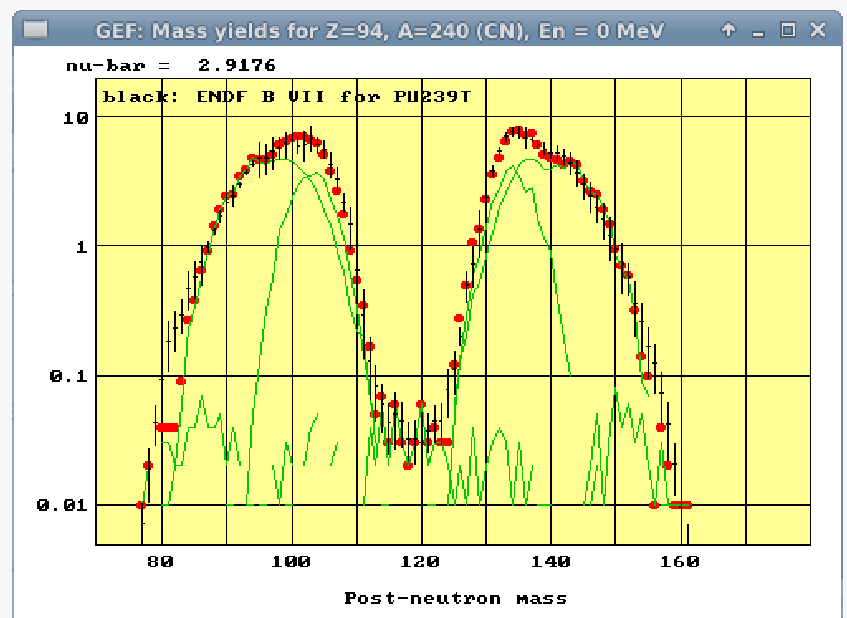
(The GEF code is described in JEF/DOC 1423, also available from www.khs-erzhausen.de.)

Calculations with perturbed parameters

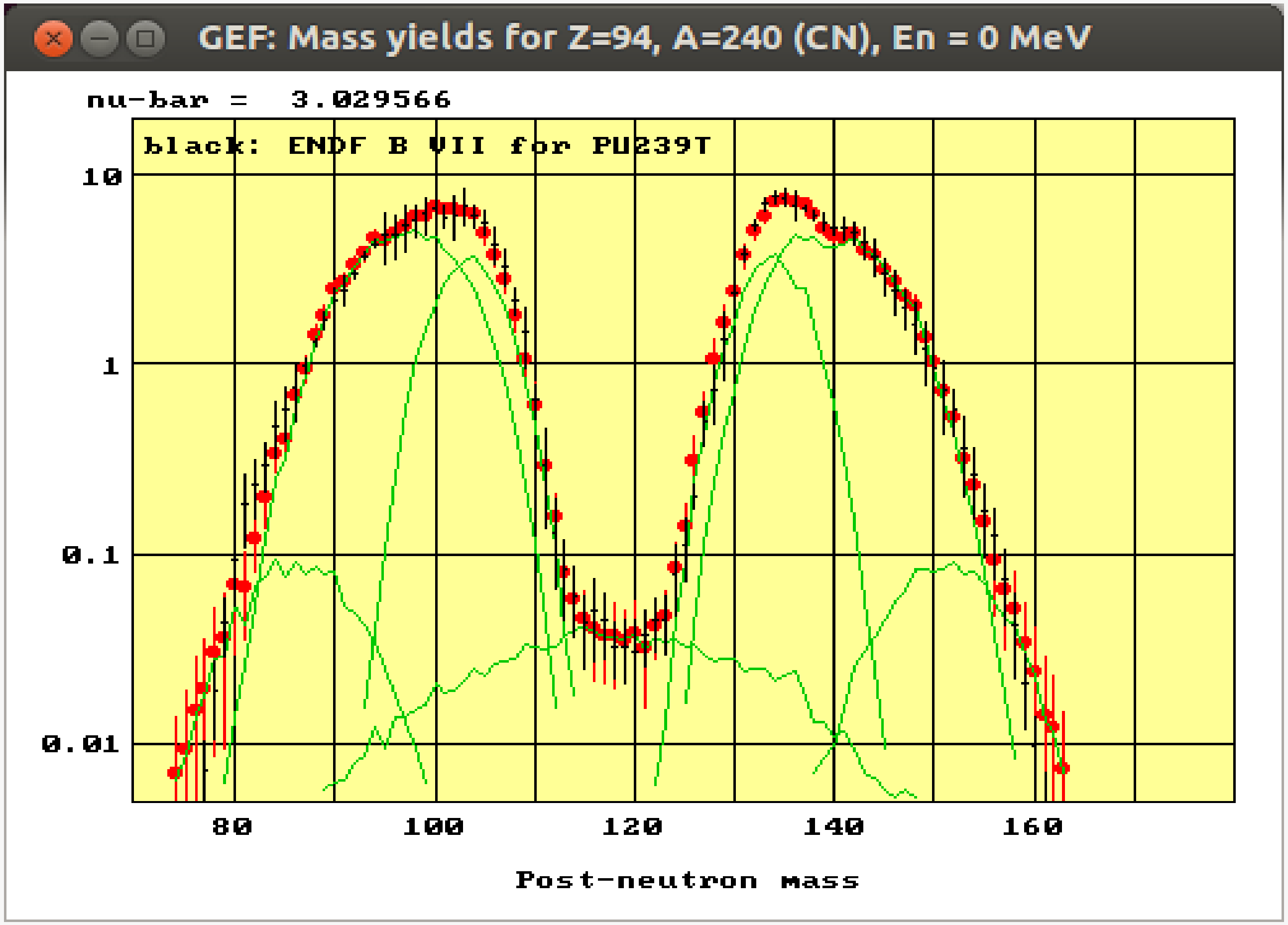








Uncertainty estimates from perturbed-parameter calculations



red: Error bars of the model calculation.
black: Error bars of the evaluated data.

Model parameters fluctuate inside their uncertainty range (deduced from the fit procedure).

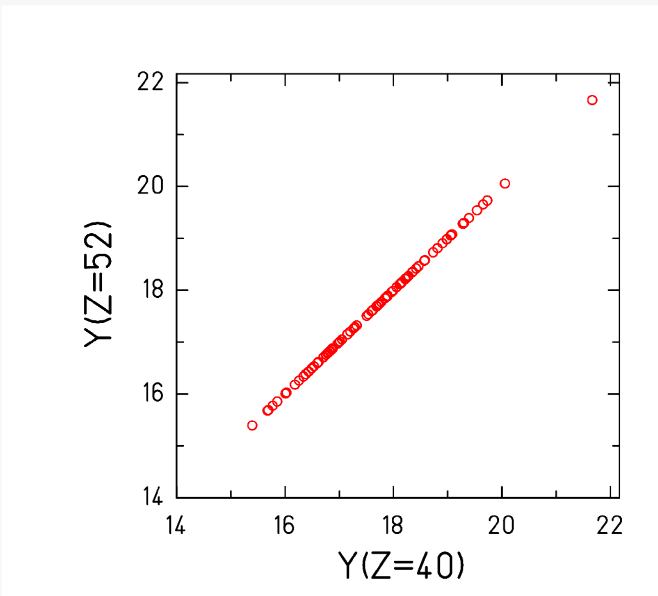
Fluctuations of the results → uncertainties of the fission observables.

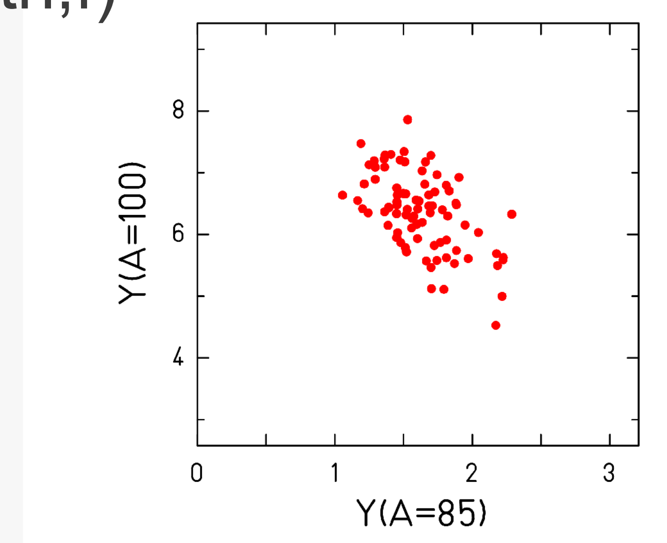
Applicable to any of the fission properties.

Correlations of fission observables

Calculations with perturbed model parameters reveal correlations of any pair of observables.

235U(nth,f)

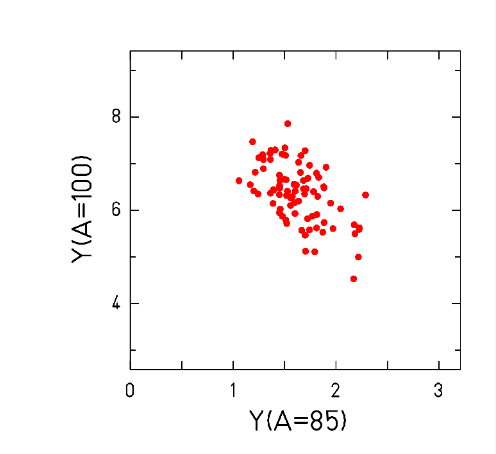




A trivial case:
two complementary elements
(Strictly correlated)

A nontrivial case:
two masses
(Slightly anti-correlated)

Establishing the covariance matrix



GEF result: Calculation with perturbed parameter values.

The covariance between two variables *x* and y is defined by:

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

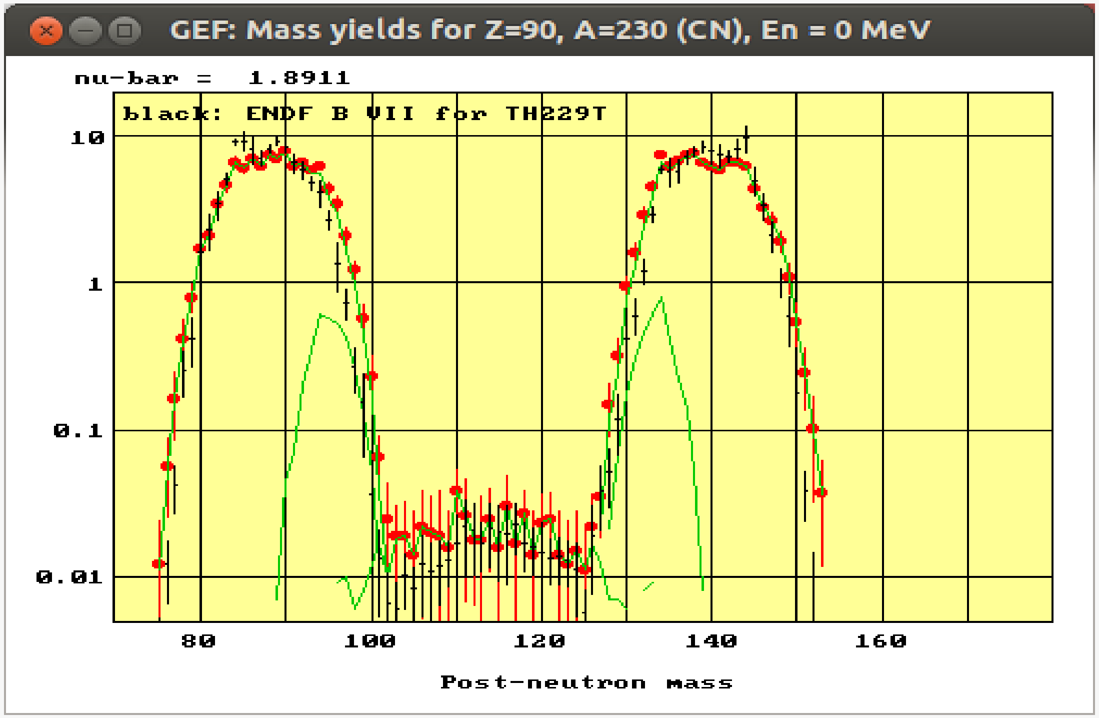
The covariance values between any two yield values *Ya* and *Yb* can be determined from the GEF calculation with perturbed parameters.
All covariance values form the covariance matrix.
The covariance matrix represents the internal logic dependences (trivial ones and model-specific ones) of GEF.

Adjustment of GEF results to partial experimental data

- Aim:
  - Fill incomplete data sets with GEF calculations
- Method:
  - Establish covariance matrix of GEF yields.
  - Merge with covariance matrix of exp. data.
  - Determine "adjusted" GEF yields.

An example:

A “bad” case:
229Th(nth,f)



- Experimental data are incomplete.
- GEF results differ from experiment.
- GEF result must be “adjusted” to experiment in order to fill the gaps..

black: evaluated data

red: GEF result (error bars from perturbed calculations)

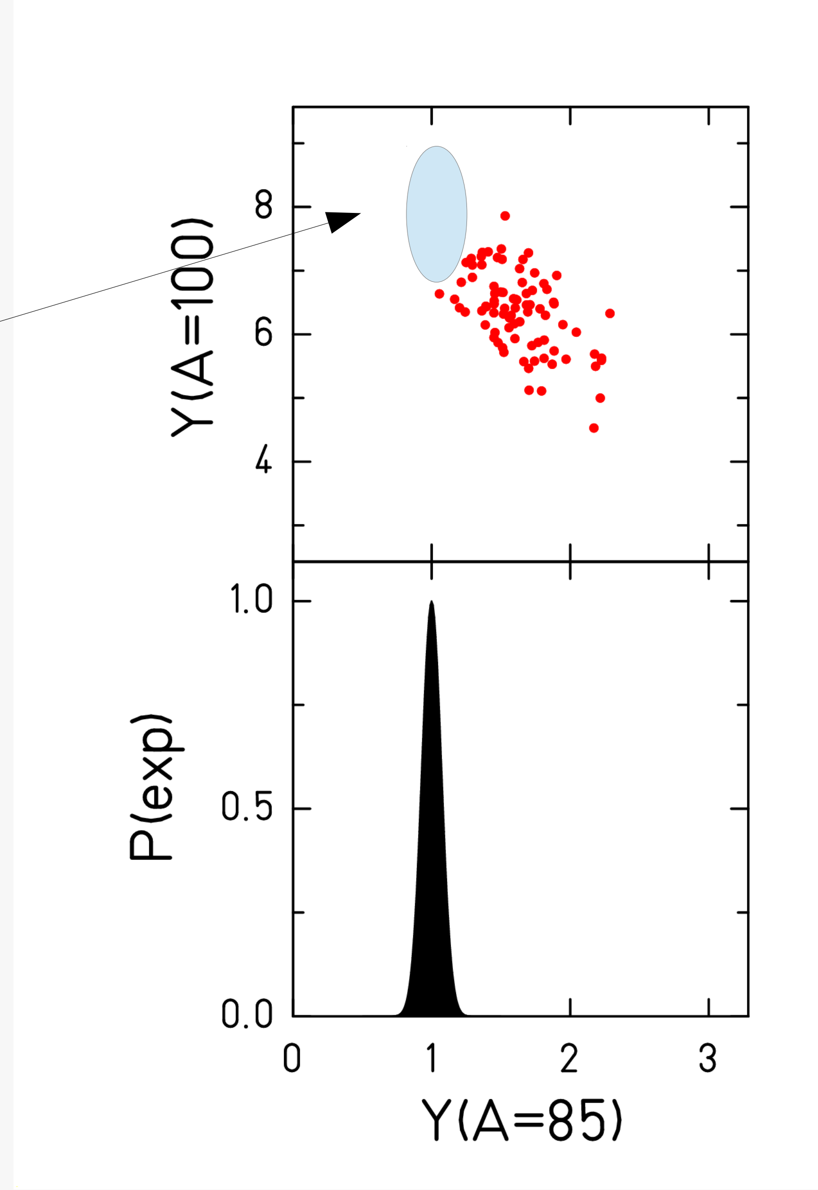
Combining GEF with experiment (schematic)

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.



Mathematics in 2 dimensions

GEF result (multivariant distribution):

$$f(x,y)=\frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}}\cdot\exp(-\frac{1}{2(1-\rho^2)}[\frac{(x-\mu_x)^2}{\sigma_x^2}\frac{(y-y\mu_y)^2}{\sigma_y^2}-\frac{2\rho(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y}])$$

Log-Likelihood:

$$L_{GEF}(x,y)=-\frac{1}{2(1-\rho^2)}[\frac{(x-\mu_x)^2}{\sigma_x^2}\frac{(y-y\mu_y)^2}{\sigma_y^2}-\frac{2\rho(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y}]$$

Experiment:

$$L_{\exp}(x)=-\frac{(x-x_m)^2}{2\sigma_{xm}^2}$$

Combined:

$$L_c=L_{GEF}+2\cdot L_{\exp}$$

Solution: search maximum of L_c with respect to x and y.

Full mathematical procedure

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

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

covariance matrix yield GEF yield

- 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: Complemented set of yields.

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.

Summary

- A new evaluation method is proposed
- General laws of quantum and statistical mechanics are respected
- Trivial and complex correlations are fulfilled
- Data are respected “as much as possible”
- Internally conflicting data are recognized
- Method relies on the “completeness” and “flexibility” of the GEF model