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Fission yield calculations with TALYS+GEF in the fast and high energy range and comparisons to experimental data

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Outline

- Why TALYS+GEF?
- A few words on the TALYS and GEF codes
- TALYS-1.6:
  - Some sample observables
  - Comparisons to experimental FY data for ^{232}Th(n,f) and ^{238}U(n,f) in the 10-33 MeV range
- Towards TALYS-1.8
  - Comparisons to FY from ^{234}U(n,f) in the 0.2-5 MeV range
  - A go on randomization of GEF parameters
  - And then?

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Motivation for TALYS+GEF

- Combine the "best" available model codes for nuclear reactions and fission

- Complement TALYS (state-of-the-art, comprehensive nuclear reaction modelling code) for Total Monte Carlo (TMC) and TENDL
  - Option to replace TANES and TAFIS in the T6 code package with GEF
  - Produce complete and consistent ENDF

- Add TALYS capabilities to GEF: handling of pre-fission stages, multi-chance fission, fission probabilities, and de-excitation

- Need analysis tool for experimental data from, e.g. IGISOL: independent fission yields from neutrons with fast reactor-like energy spectrum

(see Mattera *et al.*, NDS **119**, 416 (2014); Solders *et al.*, NDS **119**, 338 (2014), and their talks here at FIESTA)

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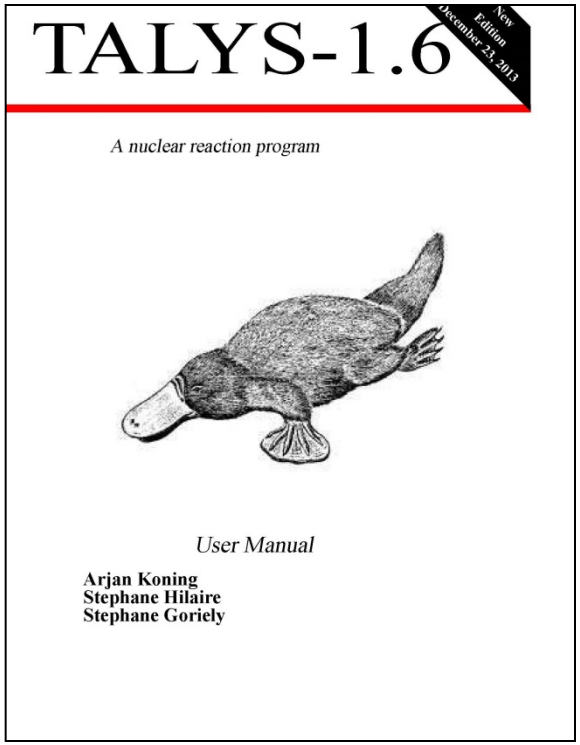
TALYS-1.6 and fission

A comprehensive nuclear model code.

Latest release: TALYS-1.6, Dec 2013 (www.talys.eu)



Fission in TALYS-1.6:

A large number of keywords can steer treatment of fission barriers, level densities, class II/III states, etc.

For the fission yields, to models are available:

`fymode=1:` Brosa model

(M.C. Duijvestijn et al, PRC 64, 014607 (2001)

`fymode=2:` GEF model based on translation of the original BASIC code to FORTRAN and with MC approach; number of samplings steered by keyword `gefran`.

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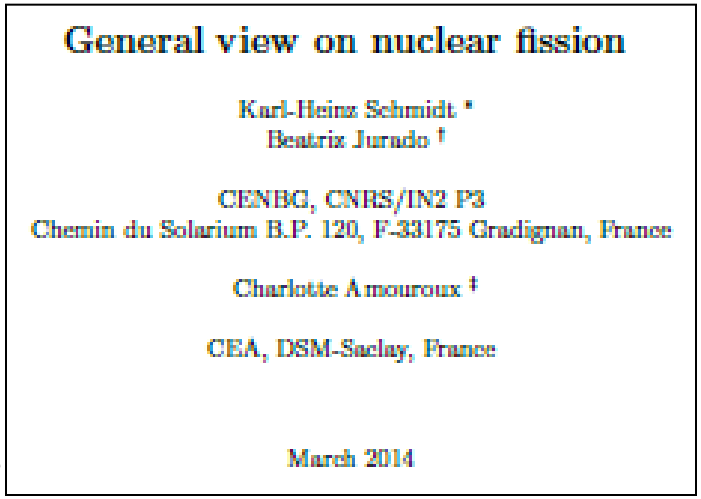
A few words on GEF

The GEF (General Fission) code is developed by Karl-Heinz Schmidt and Beatriz Jurado and described in a recent report
http://hal.in2p3.fr/docs/00/97/66/48/PDF/GEF.pdf


General view on nuclear fission

Karl-Heinz Schmidt *
Beatriz Jurado †

CENBG, CNRS/IN2 P3
Chemin du Solarium B.P. 120, F-33175 Gradignan, France

Charlotte Amouroux ‡

CEA, DSM-Saclay, France

March 2014

GEF is using **general theoretical ideas**
to describe fission **without microscopic calculations**
Hence it is rather **fast** and therefore **good for TMC**.

GEF uses **about 50 parameters** that have been adjusted to fit a large number of systems. **Several parameters and claimed uncertainties** are described in the above report, e.g., position and width of fission channels, shell effects and fragment deformation.

GEF 2012 is part of TALYS 1.6: gives yields (pre and post), nubar, nu(A) etc.

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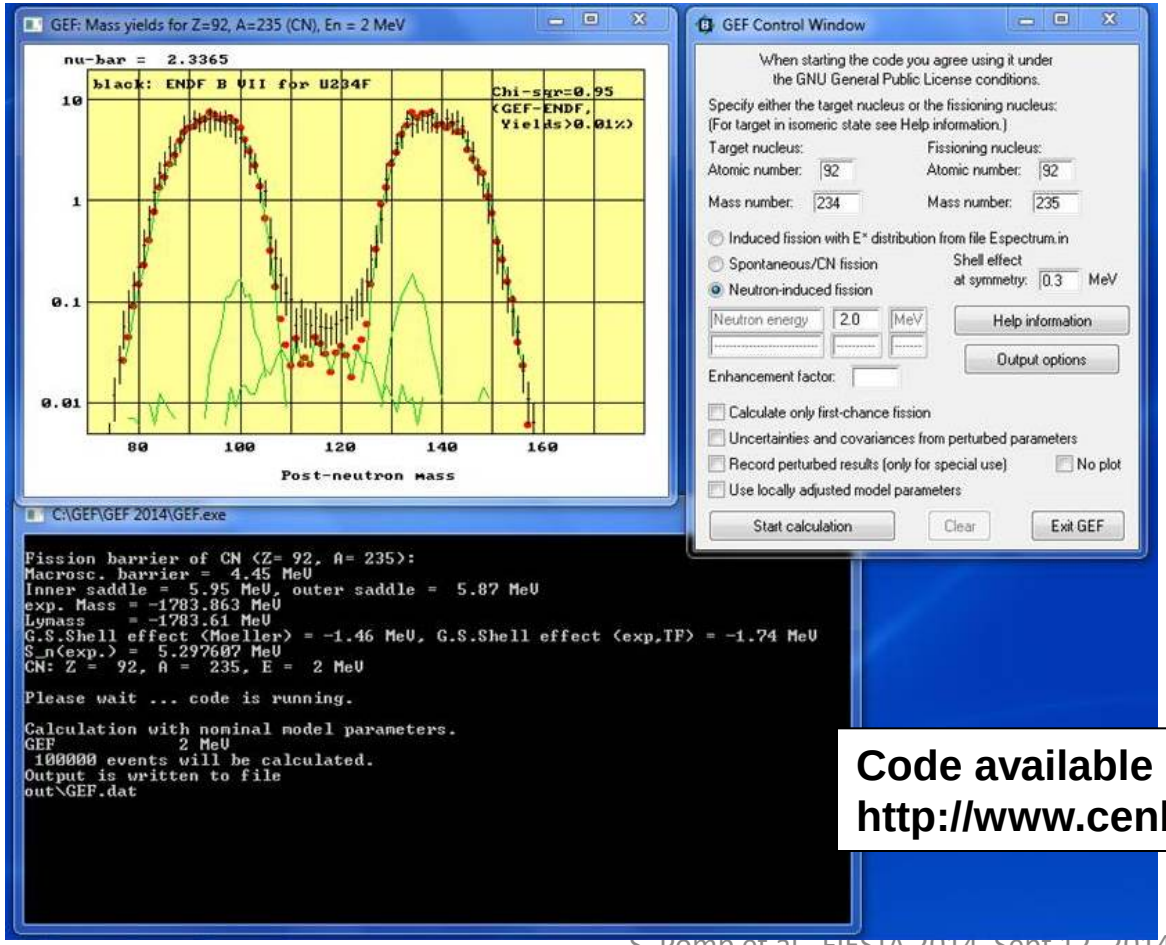
GEF – a screenshot

GEF 2014/2.1 stand-alone version:

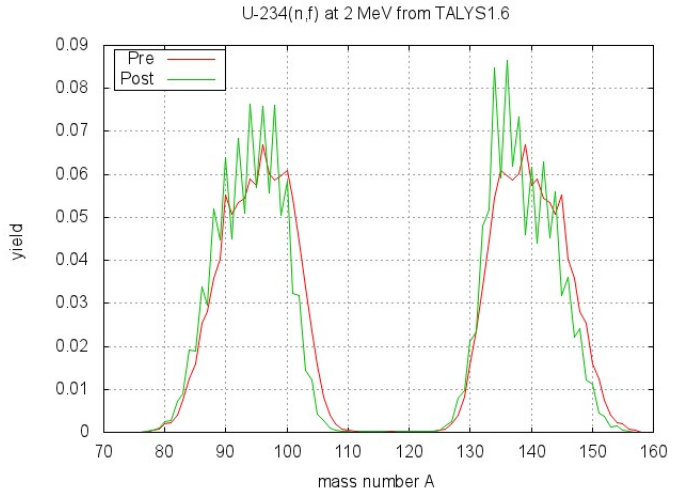


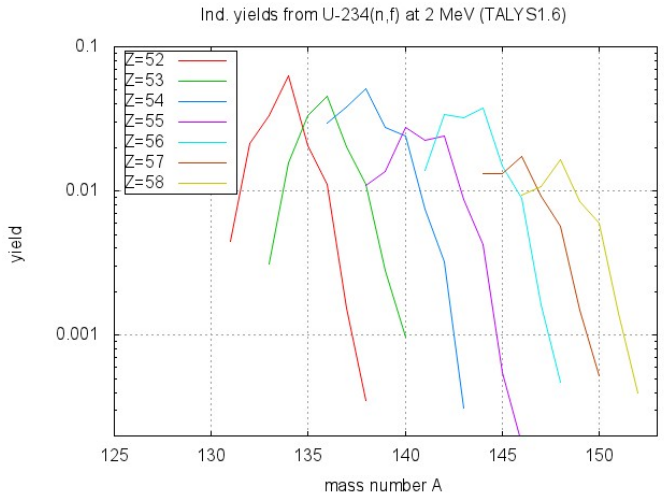
Has been validated for a large number of systems and even identified experimental problems; see JEF/DOC-1568-1573

Code available from http://www.cenbg.in2p3.fr/-GEF-

TALYS-1.6 for ^{234}U(n,f)

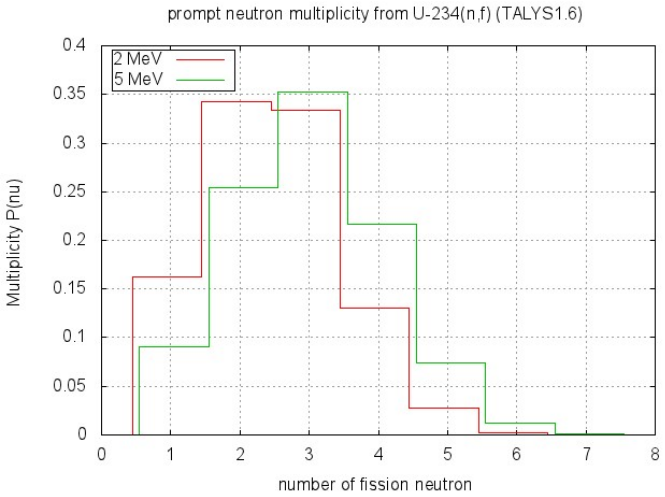
pre and post yields





independent yields

neutron multiplicities



$\bar{\nu}$ (2 MeV) = 2.5250
JEF 3.1.2: 2.6176

$\bar{\nu}$ (5 MeV) = 2.9714
JEF 3.1.2: 3.0275

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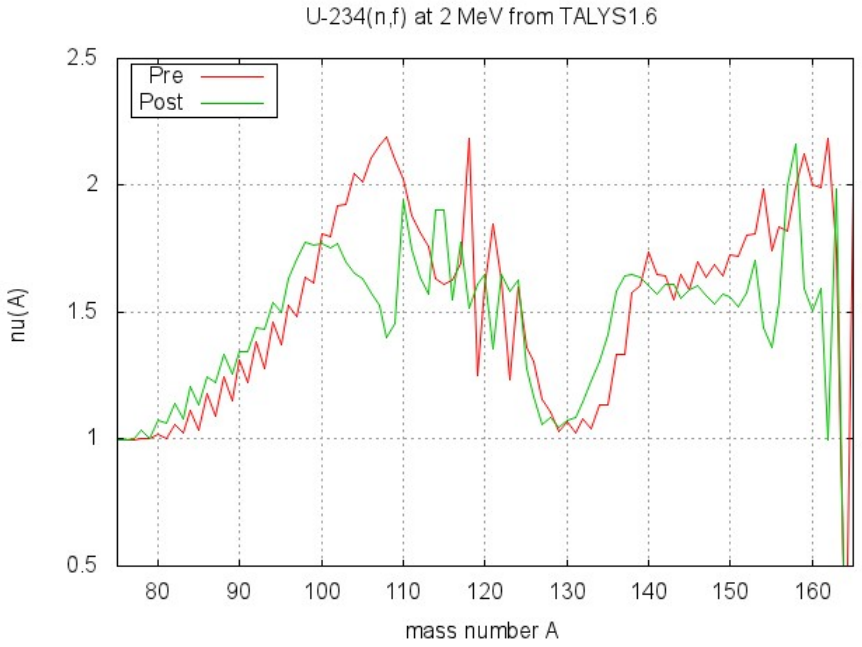
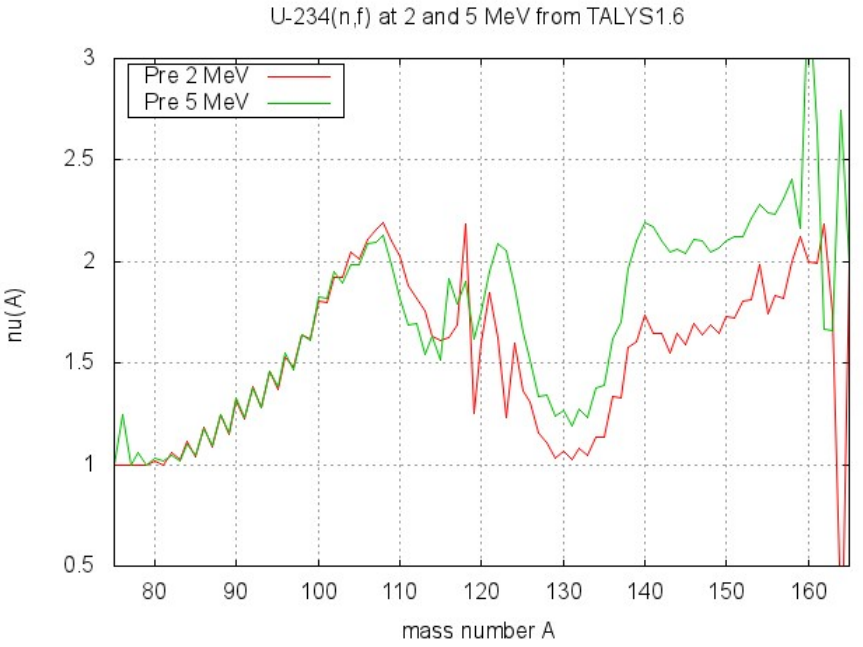
TALYS-1.6 for ^{234}U(n,f)



ν(A) pre- and post-neutron emission



ν(A) at 2 and 5 MeV (post)

See Al-Adili et al., NDS **119**, 342 (2014), and PhD thesis Uppsala University 2013.

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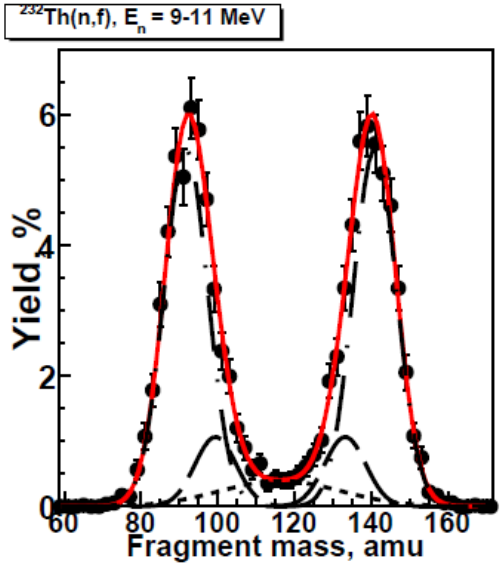
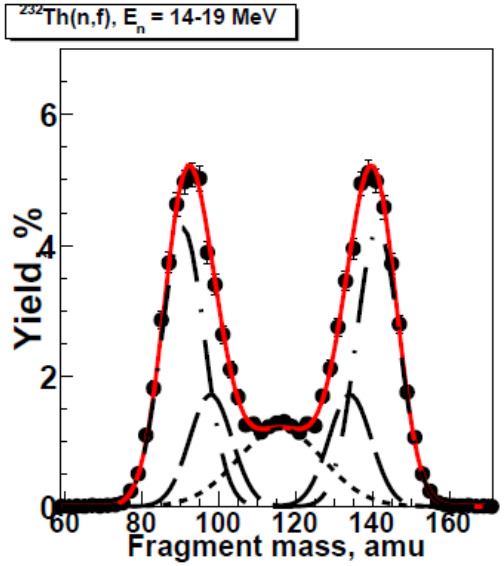
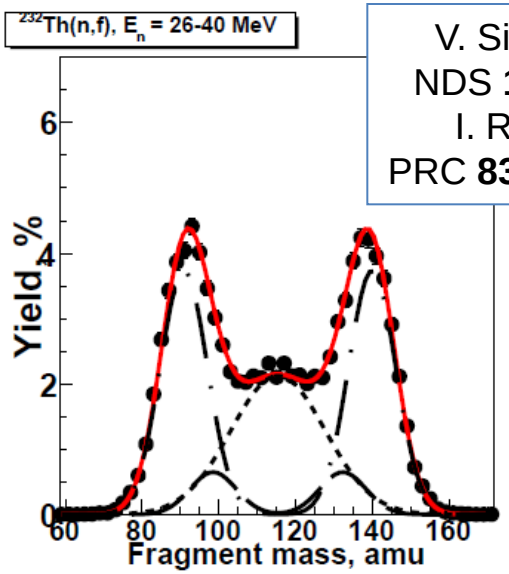
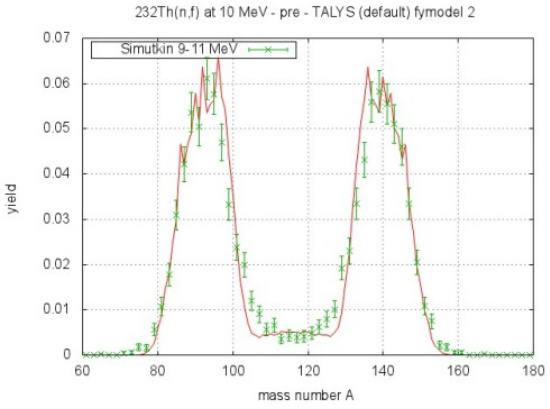
^{232}Th(n,f); E_n = 9 to 40 MeV

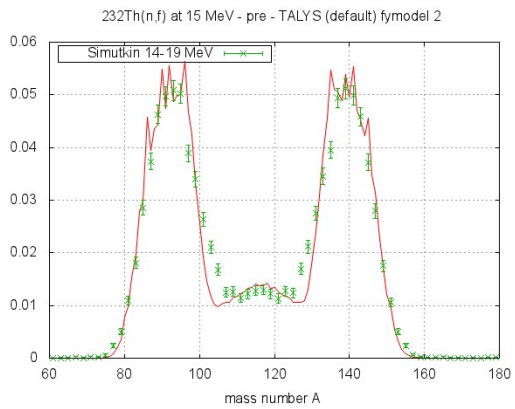


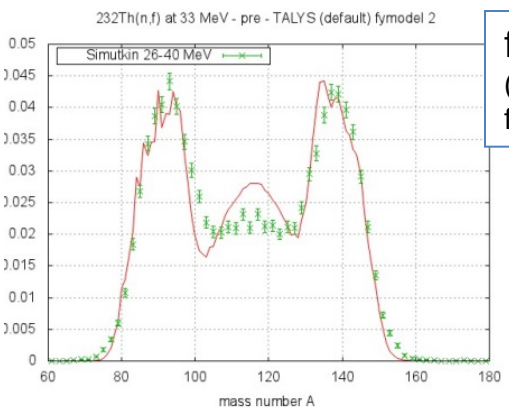




V. Simutkin et al.,
NDS **119**, 331(2014)
I. Ryzhov et al.,
PRC **83**, 054603 (2011)

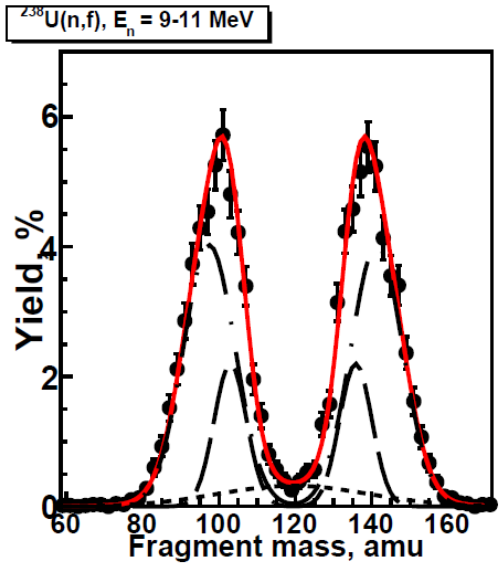


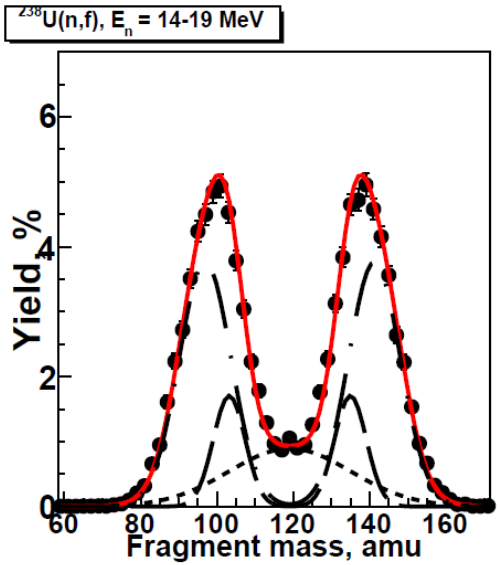


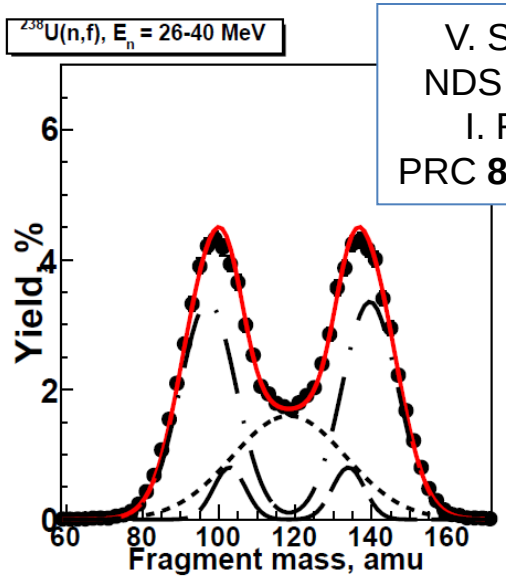


fymodel = 2
(default parameters for Th-232)

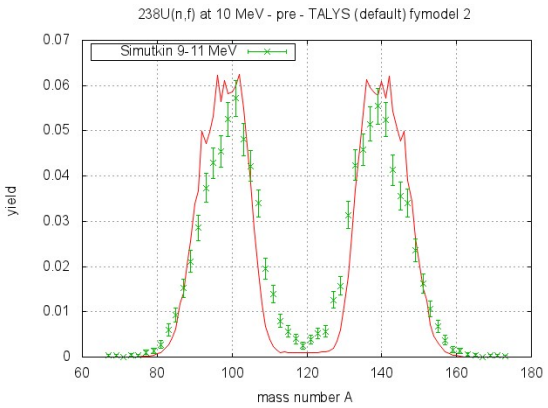
^{238}U(n,f); E_n = 9 to 40 MeV

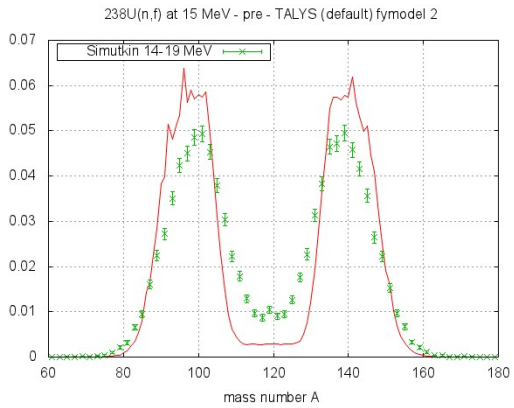


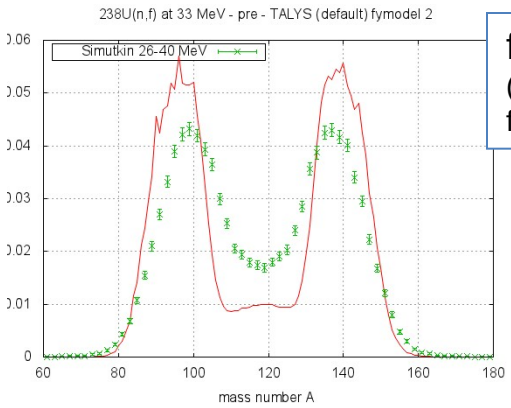




V. Simutkin et al.,
NDS **119**, 331(2014)
I. Ryzhov et al.,
PRC **83**, 054603 (2011)







fymodel = 2
(default parameters for U-238)

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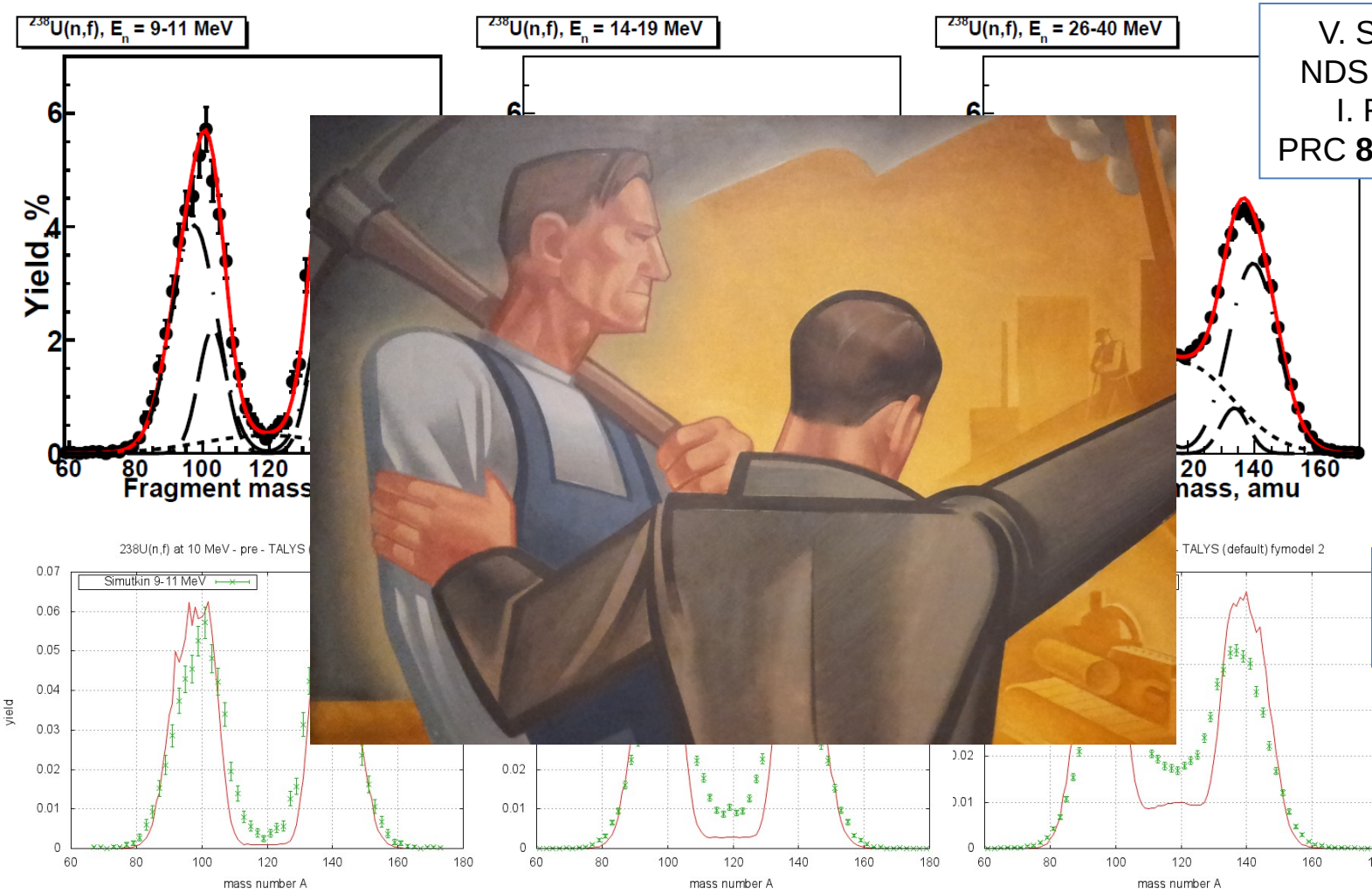
^{238}U(n,f); E_n = 9 to 40 MeV



V. Simutkin et al.,
NDS **119**, 331(2014)
I. Ryzhov et al.,
PRC **83**, 054603 (2011)

fymodel = 2
(default parameters for U-238)

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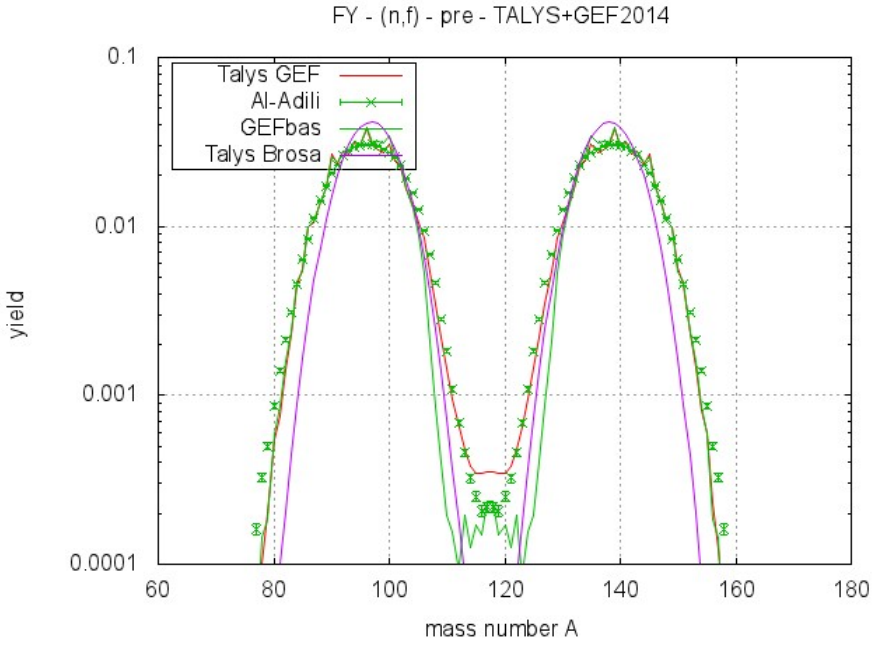
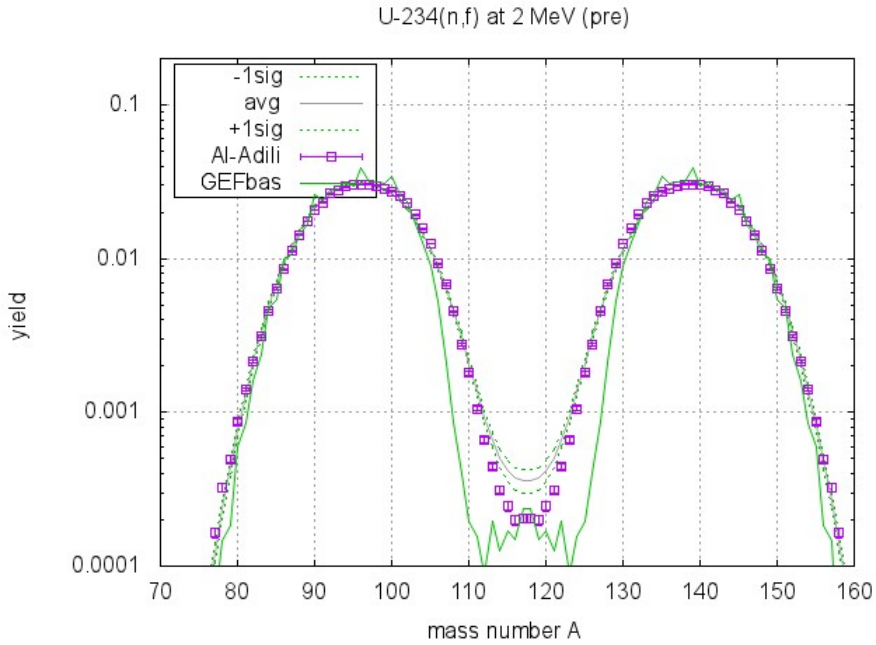
TALYS + GEF 2014/2.1

Use **latest Fortran translation (GEFSUB)** of the GEF fission code within TALYS 1.6:



Comparison with GEF (Basic) and Brosa model in Talys



TALYS + GEF2014 and randomized Parameters (250 runs); adjusted to exp. resolution

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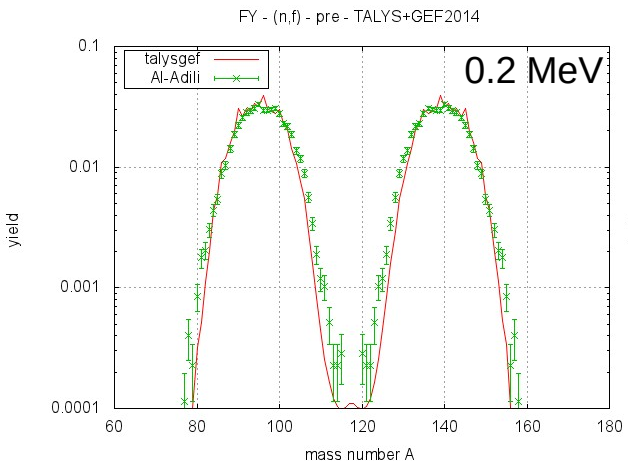
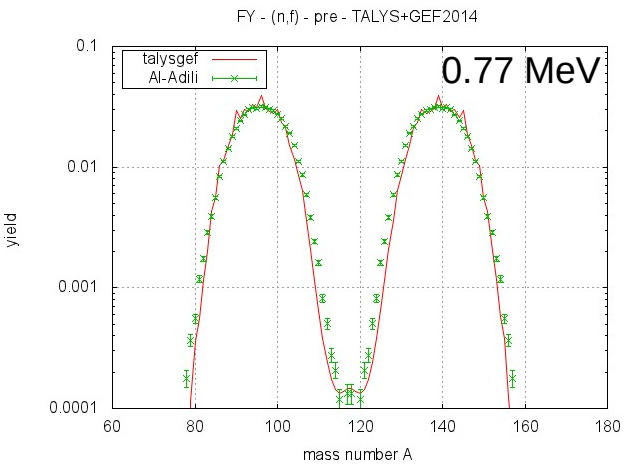
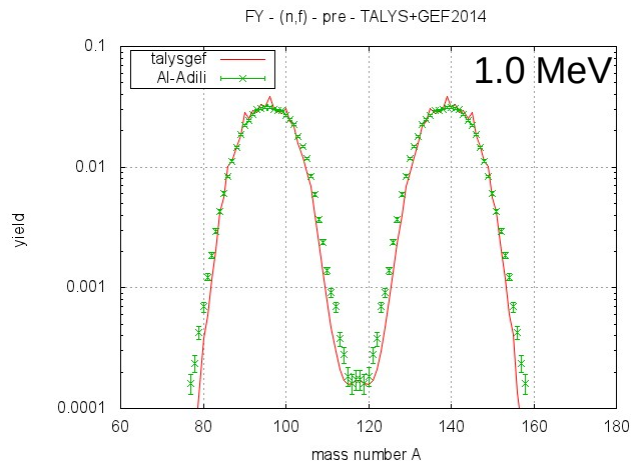
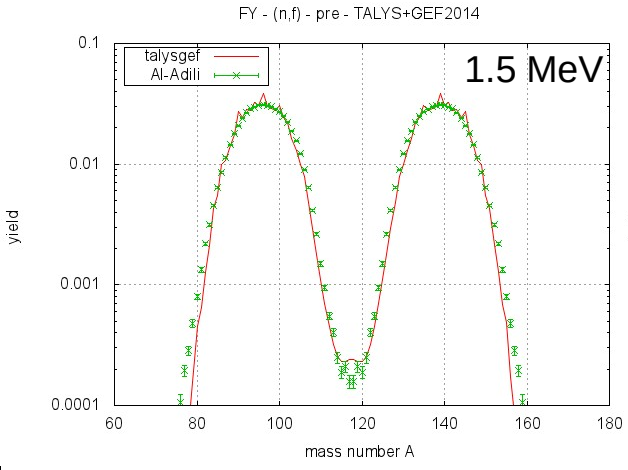
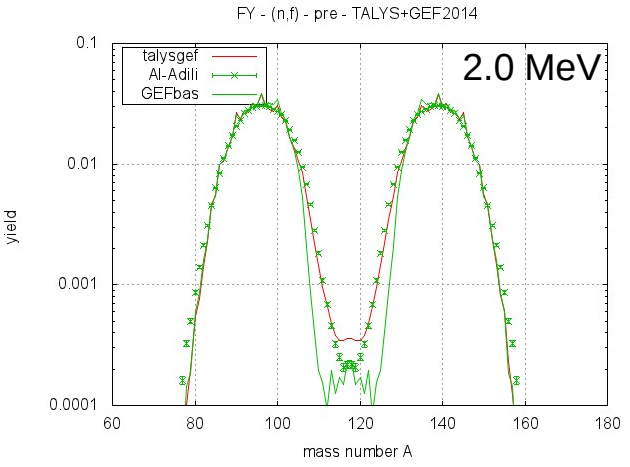
TALYS+GEF2014 for ^{234}U(n,f)

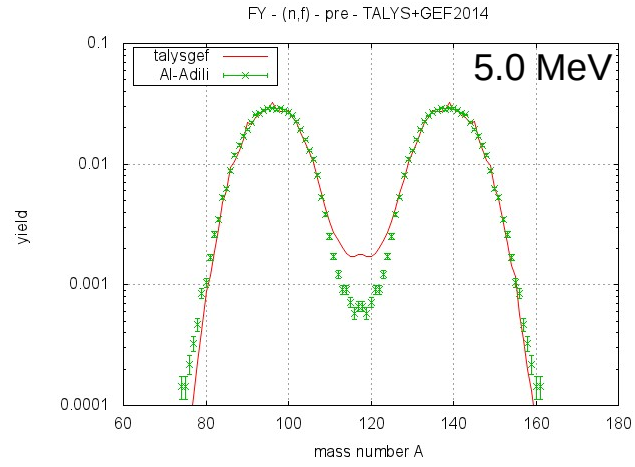










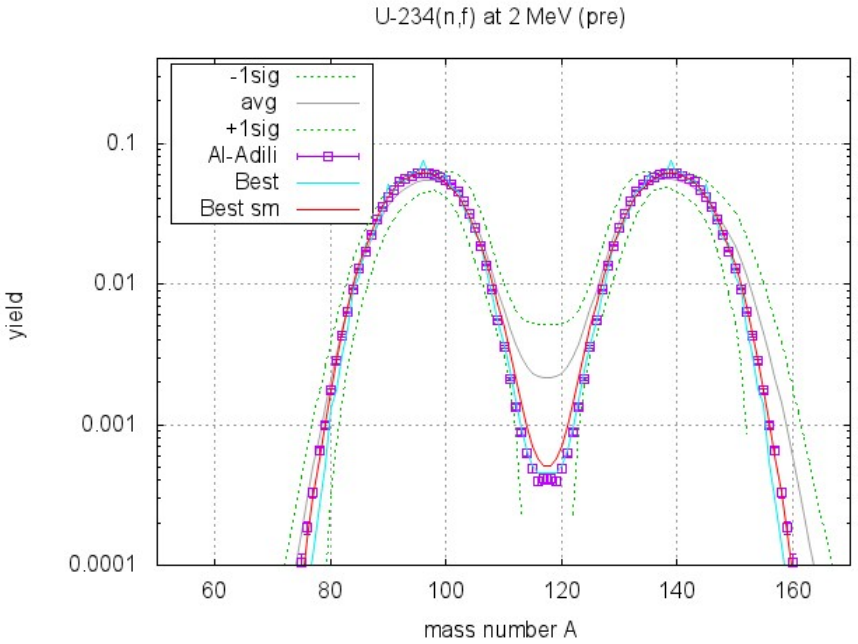


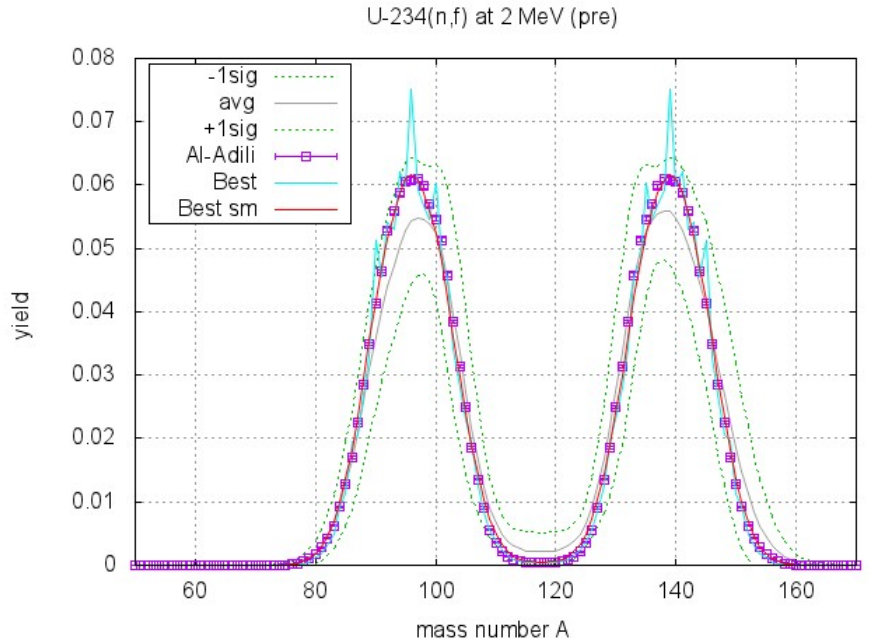
Experimental data from PhD thesis of Ali Al-Adili, Uppsala University 2013.

Try randomizing GEF parameters for ^{234}U(n,f) at E_n=2 MeV

500 TALYS+GEFSUB runs with randomization of 18 GEF parameters

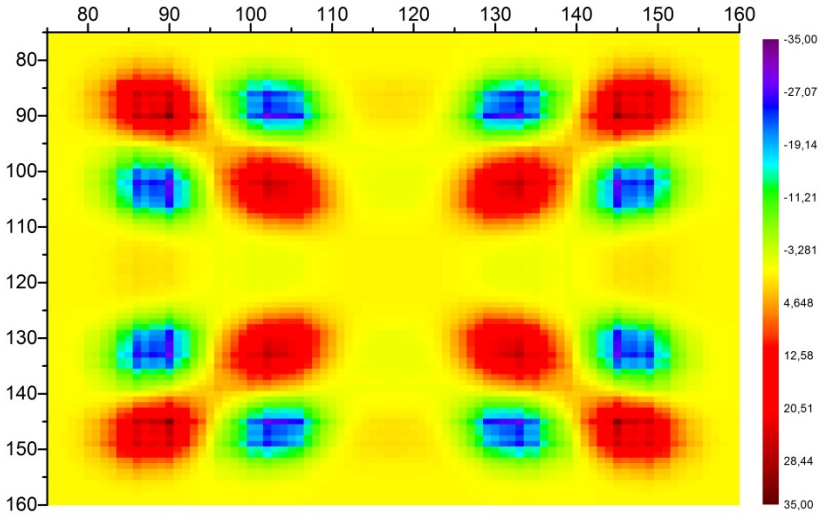
(10 times the uncertainties as given in GEF report from April 2014)



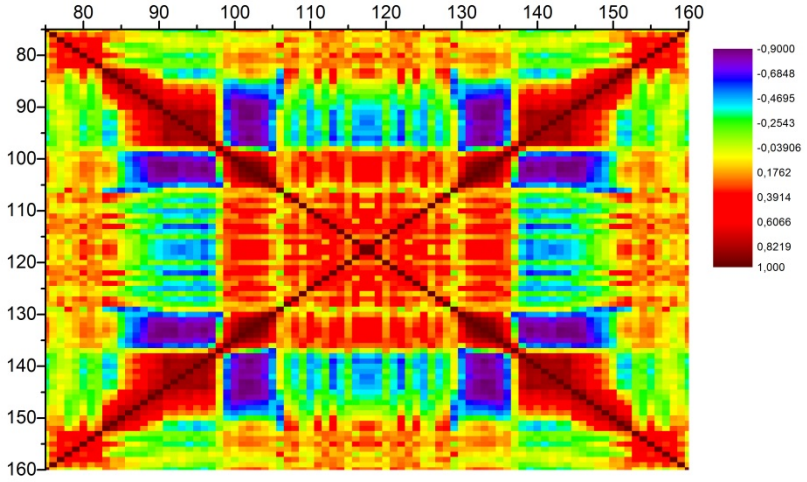


red curve: best TALYS+GEF run; adjusted to exp. resolution (4.5 AMU)

Covariances …



250 runs with TALYS+GEF2014 for ^{234}U(n,f) using parameter uncertainties from K.-H. Schmidt et al.



Correlation matrix (dito); dominated by position of S2 mode

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Under construction for TALYS 1.8

- GEFSUB returns (Z_{ff}, A_{ff}, E_x, J) arrays, i.e. for each fission fragment the J-dependent excitation energy grid, before neutron emission.
- At the end of a "conventional" TALYS calculation, i.e. when the nuclear structure arrays for the actinides can be flushed, a loop over all fission fragments is performed, still inside the same TALYS run, to deplete all excitation energy grids of these fission fragments. This gives:
  - Post-neutron FY for each Z,A
  - Nu as function of number of neutrons, P(nu), fission product, nu(Z,A), and average number of prompt fission neutrons, nubar.
  - The same for gamma's (and charged particles for high energies)
  - PFNS and PFGS, etc.
  - ……but this time calculated with the full Hauser-Feshbach and pre-equilibrium models of TALYS, including all flexibility for adjustment, optimization and covariances.
- Already present in TALYS: JEFF-3.1.1 Radioactive Decay Data File:
  - Independent and cumulative yields
  - Feeding of any isomer, including beta delayed precursors

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Acknowledgements

Special thanks to Karl-Heinz Schmidt and Beatriz Jurado for their tireless efforts to constantly improve the GEF code and even providing a Fortran source code ☺

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- **The Swedish Radiation Safety Authority**

Thanks!