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Fission yield calculations with TALYS/GEF

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Motivation for this work

- Complement TALYS (state-of-the-art, comprehensive nuclear reaction modelling code) for 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 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.*, ND2013; Solders *et al.*, ND2013)

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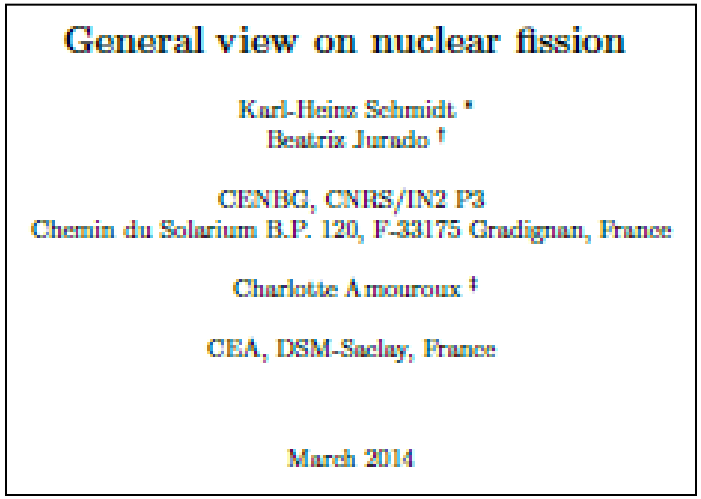
Why GEF?

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

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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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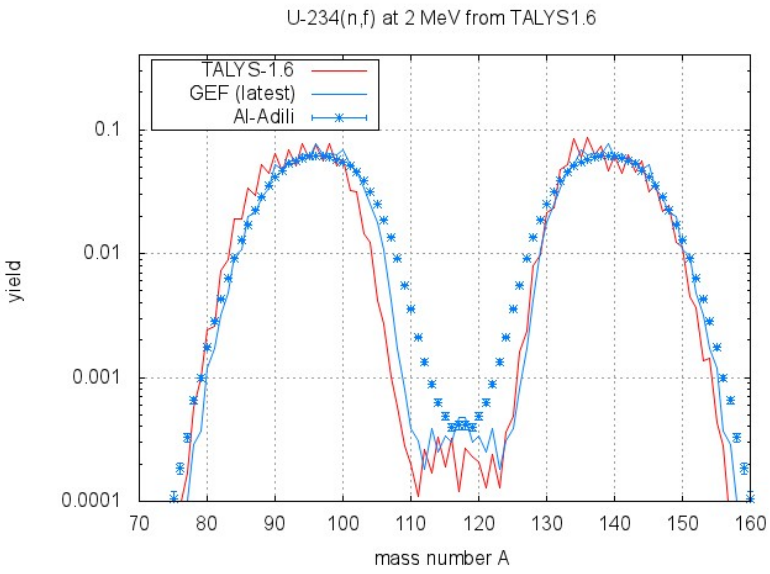
TALYS + GEF: TALYS-1.6

- Vasily Simutkin and Michail Onegin have translated part of the Freebasic code GEF (by K.H. Schmidt and B. Jurado) into Fortran
- Done for TALYS-1.6:
  - FY as function of Z, N, A (pre-neutron and post neutron emission)
  - P(nu)
  - nubar(Z,A) and nubar total
- Next TALYS version: fission neutron and gamma spectra
- GEF starts from a certain excitation energy
- TALYS provides all excitation energies and fission probabilities for all residual nuclides: multi-chance fission

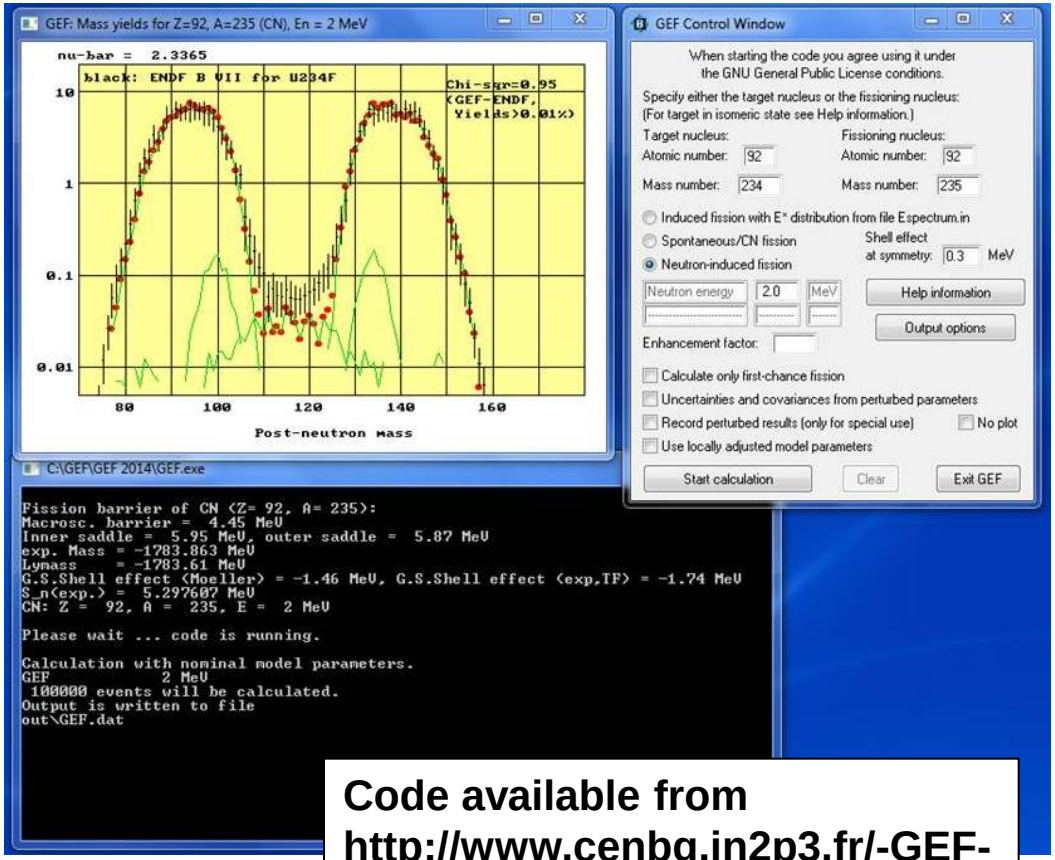
TALYS 1.6 and GEF

TALYS1.6 with GEF 2012



Exp. Data from Al-Adili et al.
(PhD thesis 2013, ND2013)

GEF 2014/2.1 stand-alone version:



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

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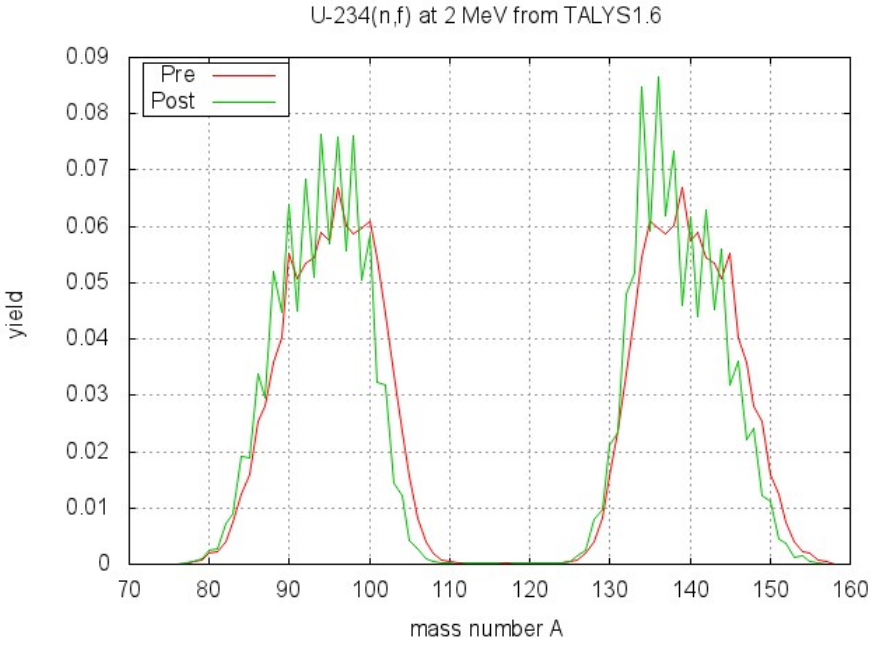
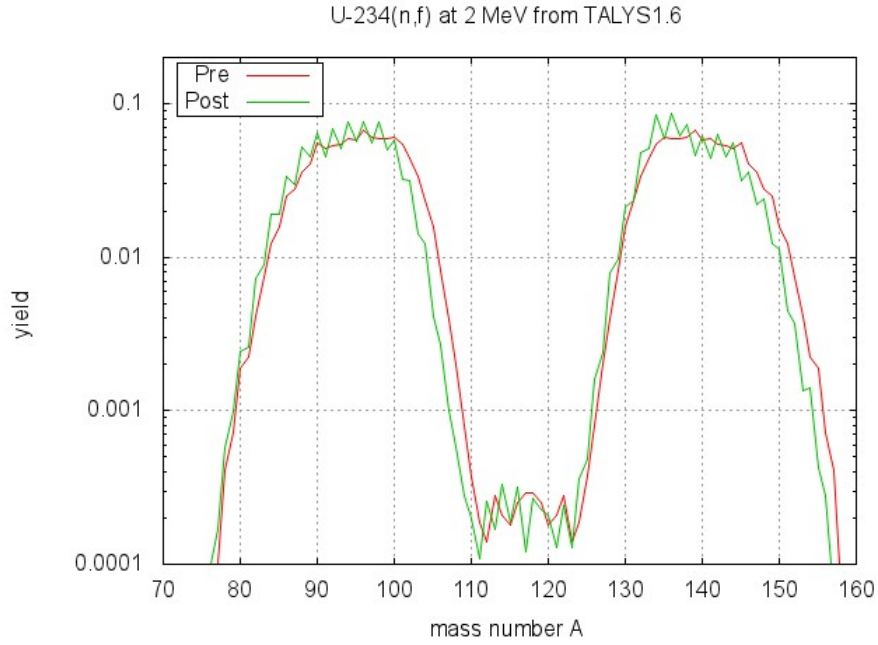
TALYS-1.6 for ^{234}U(n,f)





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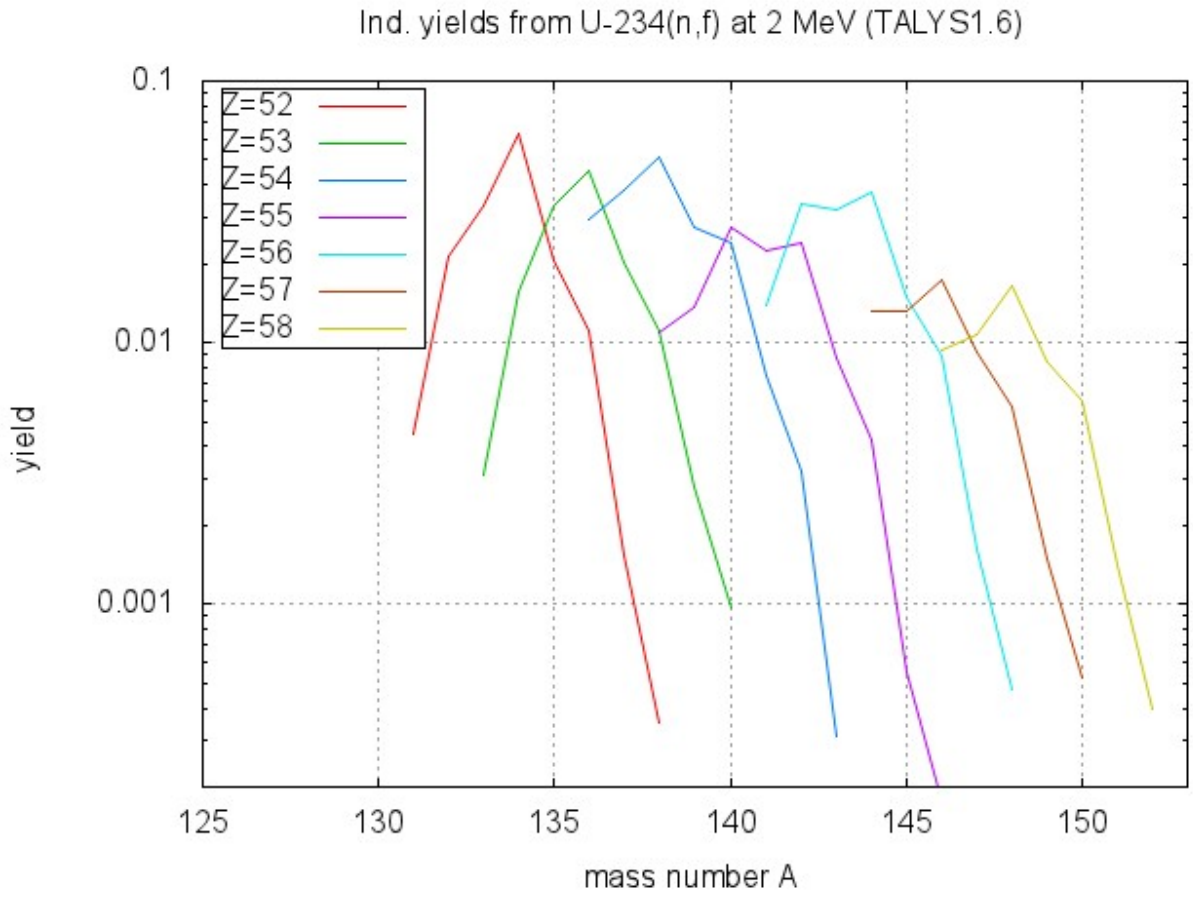
Independent yields



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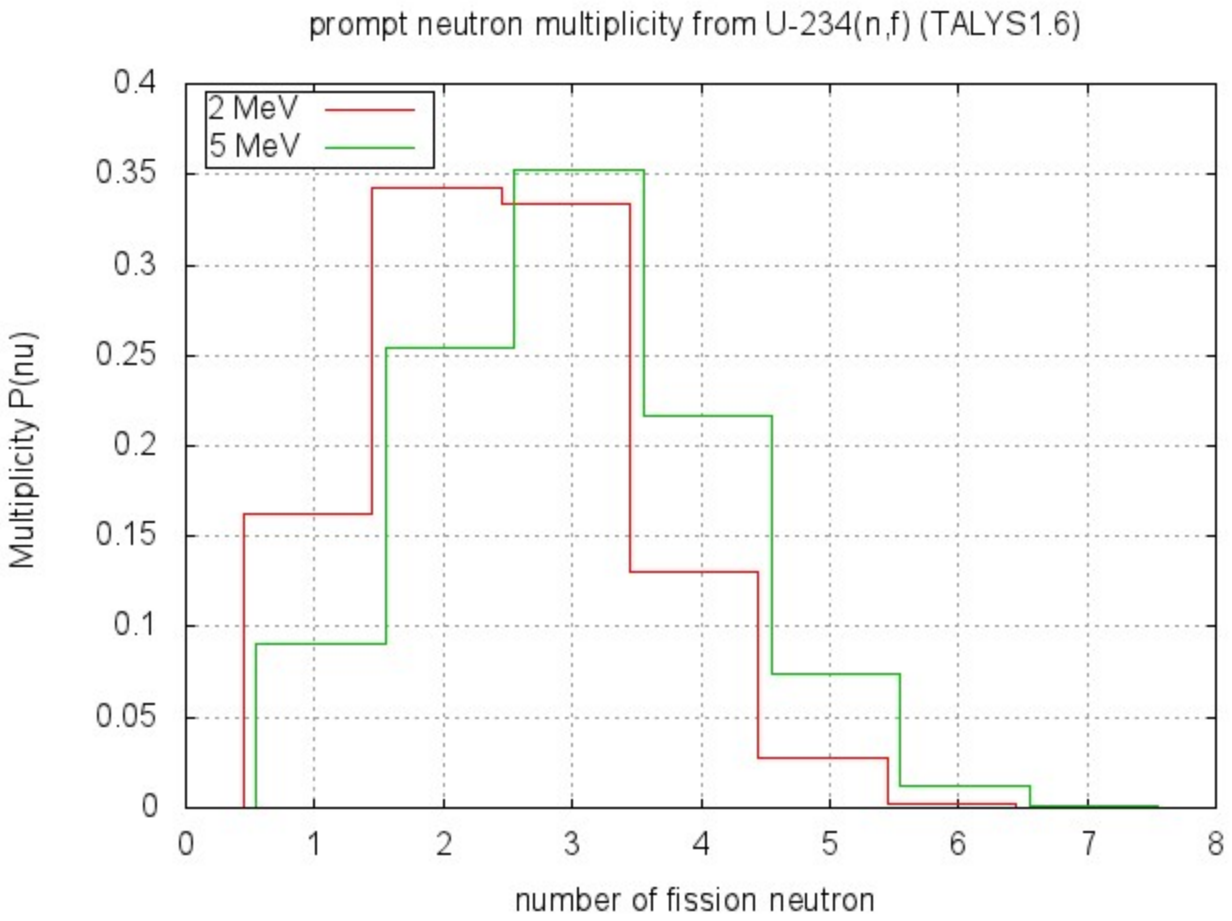
Neutron multiplicity



$\bar{\nu}$ (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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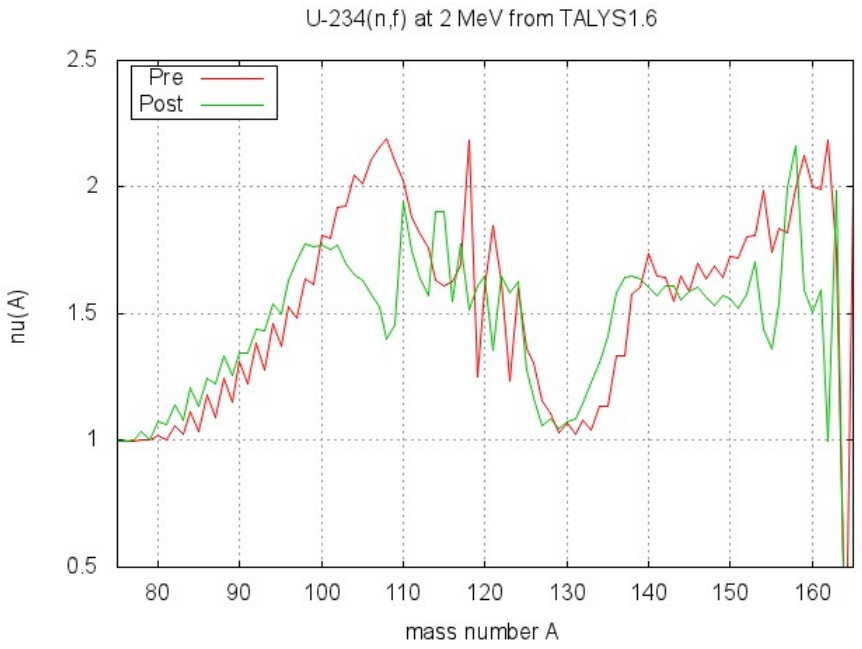
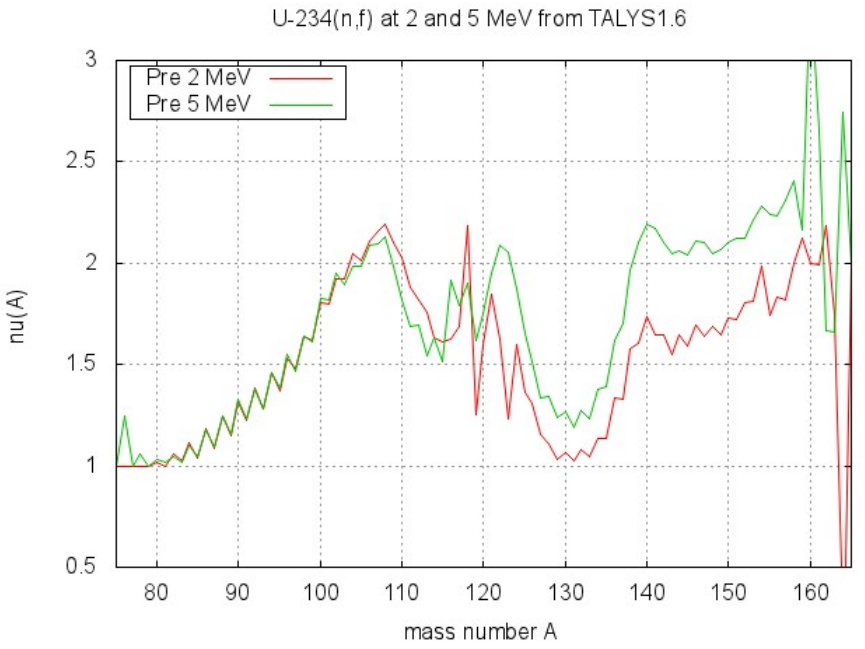
TALYS-1.6 for ^{234}U(n,f)



ν(A) pre- and post-neutron emission



ν(A) at 2 and 5 MeV (post)

See Al-Adili et al., ND2013 proceedings, arXiv:1304.2278

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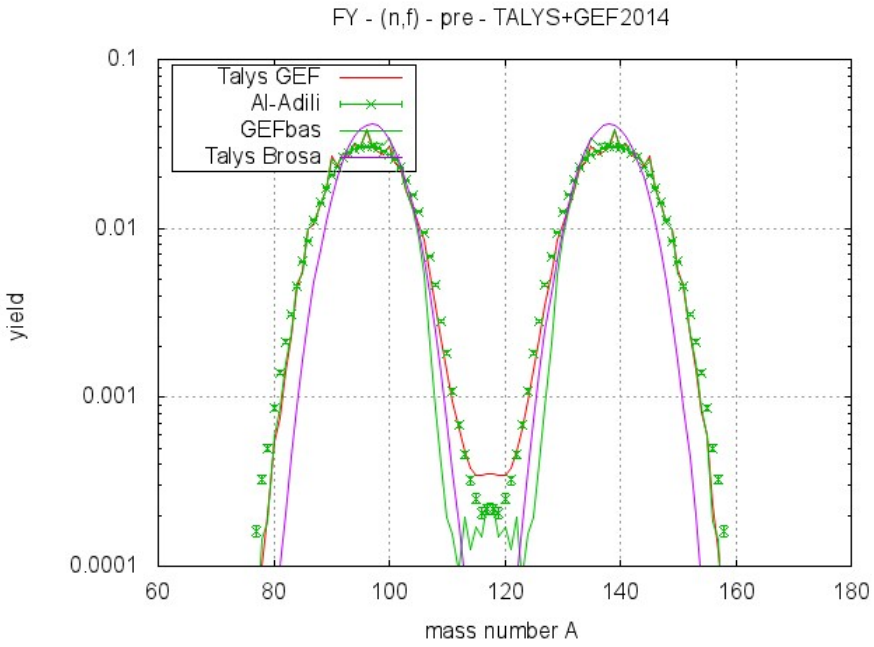
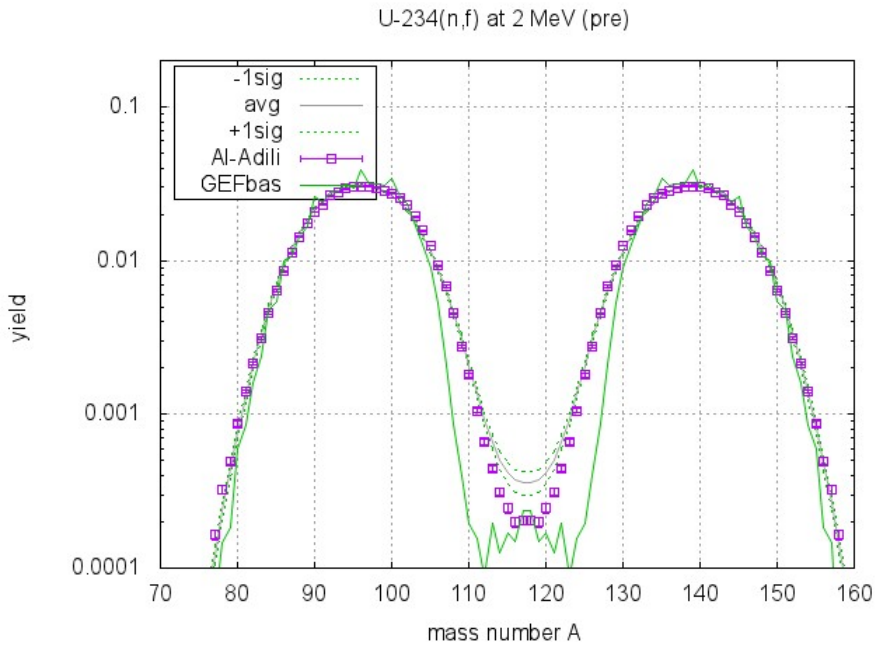
TALYS + GEF 2014/2.1

Use Fortran translation of the GEF fission code in 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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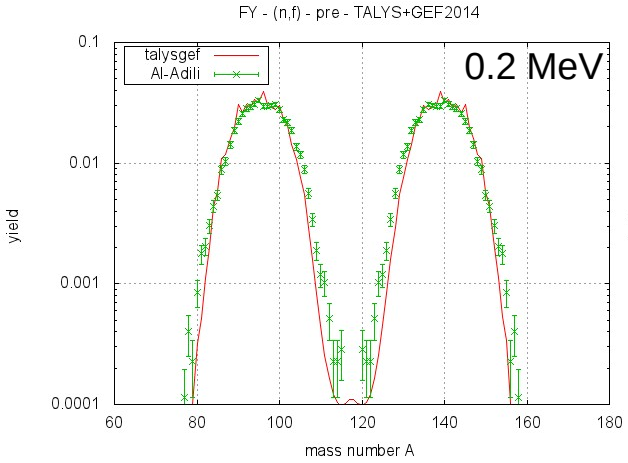
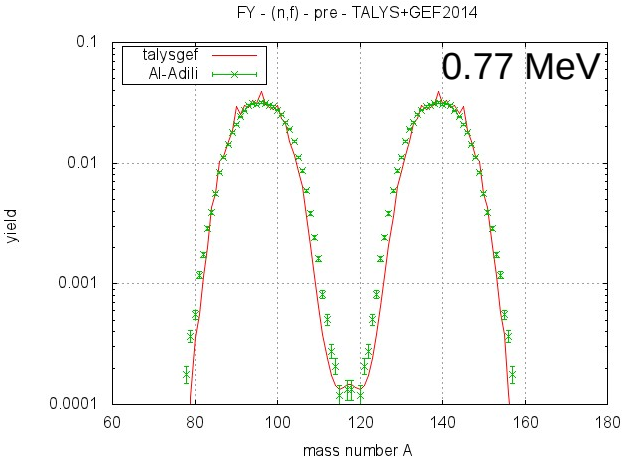
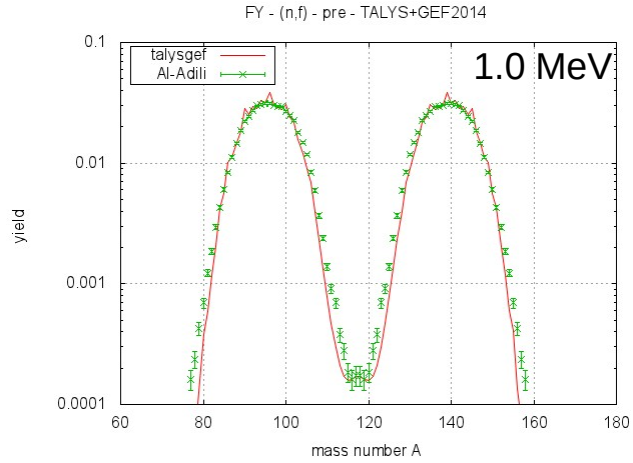
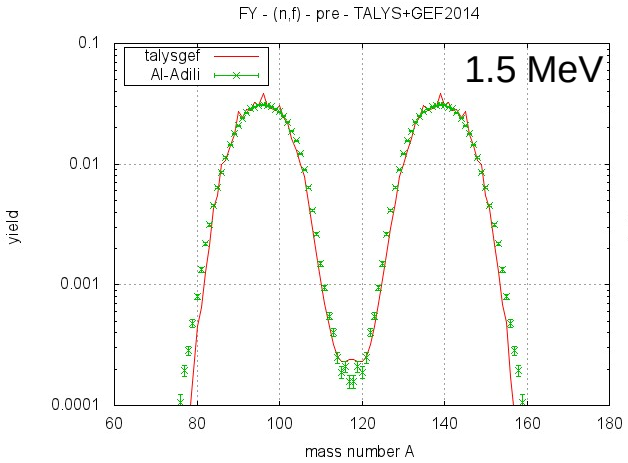
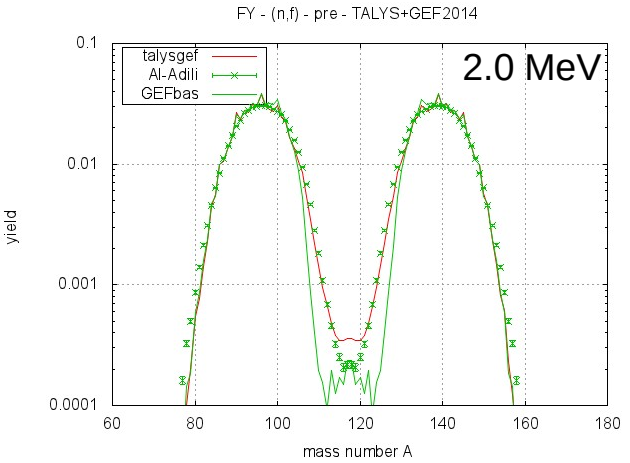
TALYS+GEF2014 for ^{234}U(n,f)

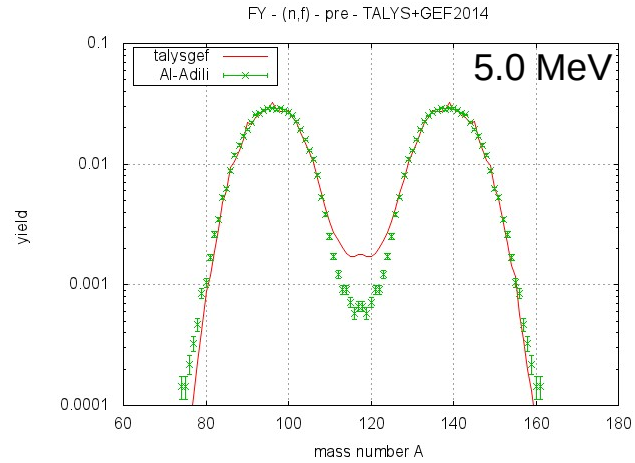












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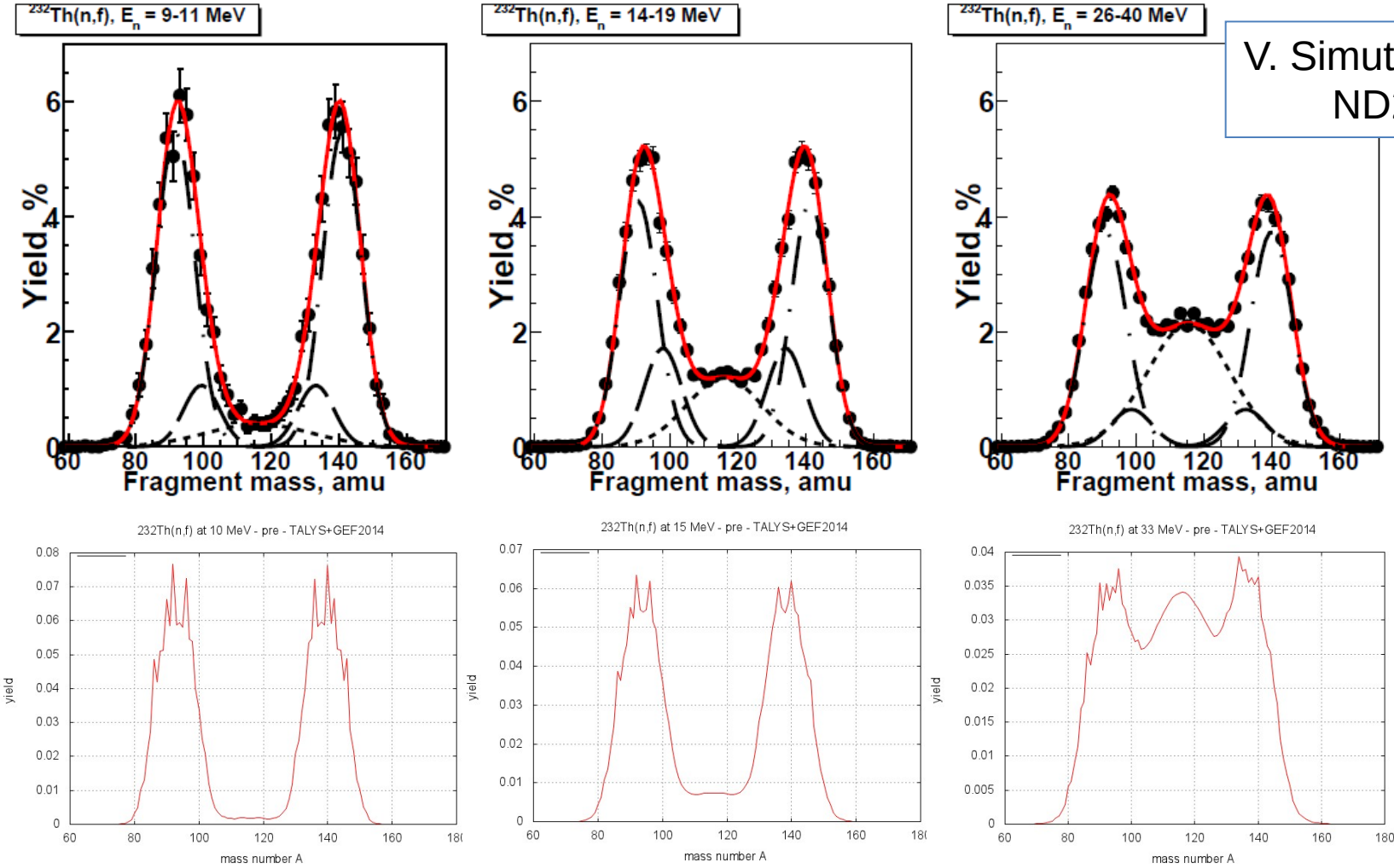
^{232}Th(n,f)

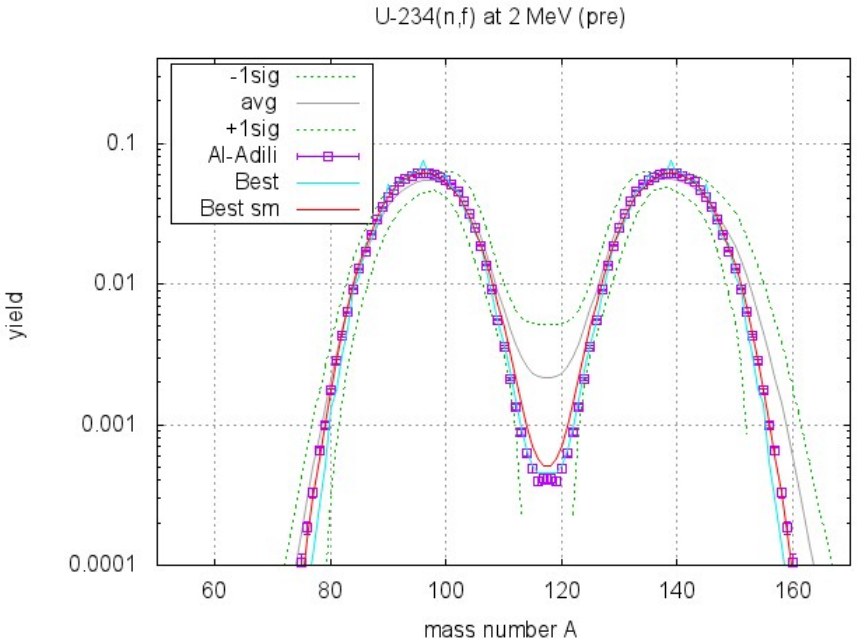


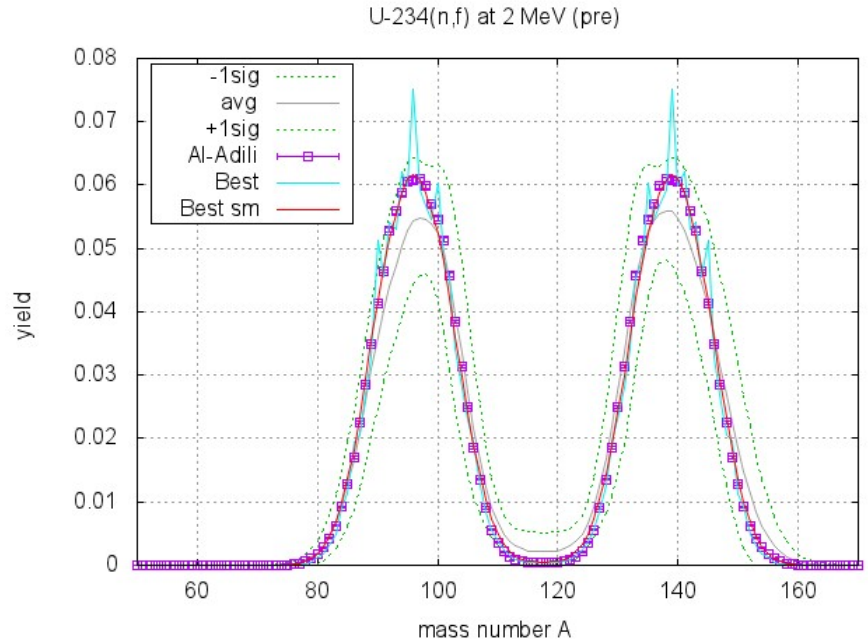
V. Simutkin et al., ND2013

Try randomizing parameters …

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)

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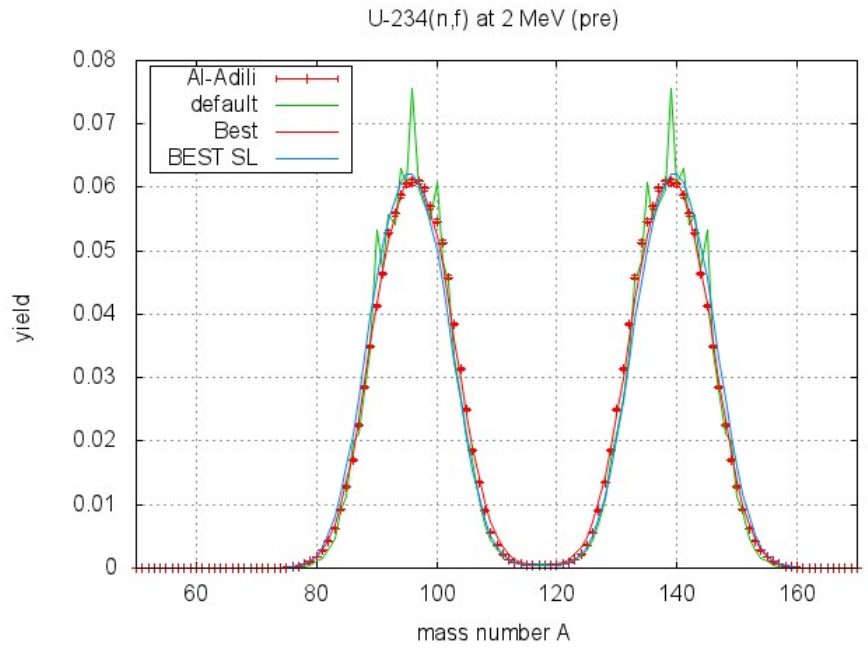
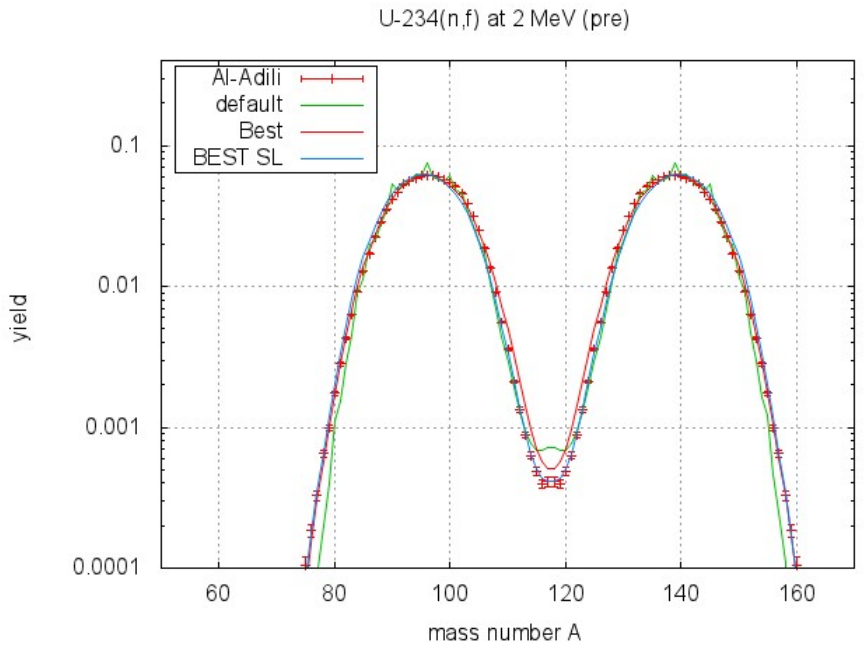
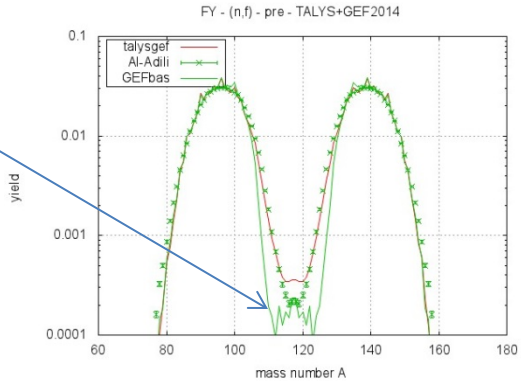
TALYS+GEF2014: best fits in sym. region





- TALYS+GEF (folding) better than GEF MC
- Adjusting parameters can further improve
- Note: GEF (stand alone)
  uses global set of parameters



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So ...

... there is (of course) room for improvement but:

- GEF (stand-alone) has been **successfully validated** for a large number of systems and even identified experimental problems (see JEF/DOC-1568 – 1573)
- TALYS/GEF results are very promising and open up for **a more complete TALYS code** (TKE, TXE, nubar, nu(A), ...) that can be used, e.g., for TENDL and fuel cycle TMC.

Under construction for next TALYS

- Karl-Heinz Schmidt provides FORTRAN subroutine GEFSUB
- 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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•EC within CHANDA and ERINDA