



# 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)



# 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>

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.

## General view on nuclear fission

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CEA, DSM-Saclay, France

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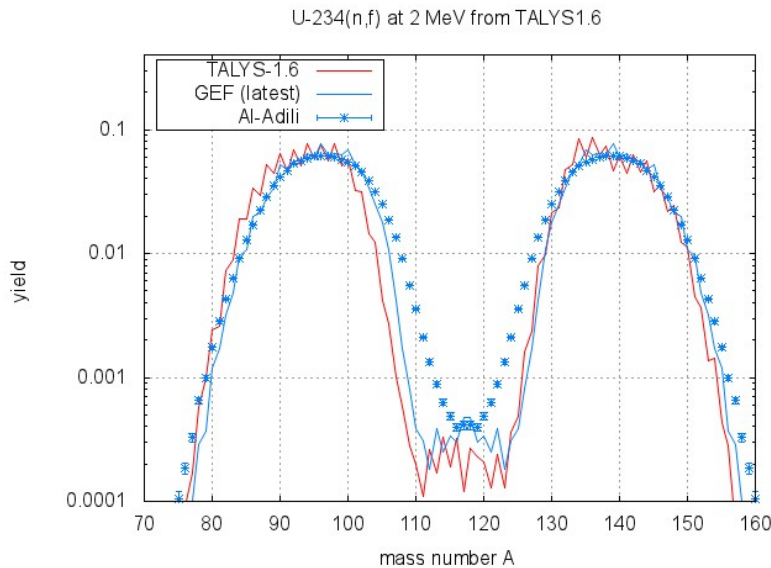
# TALYS + GEF: TALYS-1.6

- 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)
  - $\bar{\nu}(Z,A)$  and  $\bar{\nu}$  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:

GEF Mass yields for Z=92, A=235 (CN), En = 2 MeV

nu-bar = 2.3365

black: ENDF B VII for U234F

Chi-sqr=0.95  
 GEF-ENDF  
 Yields>0.01%

Post-neutron mass

GEF Control Window

When starting the code you agree using it under the GNU General Public License conditions.

Specify either the target nucleus or the fissioning nucleus: (For target in isomeric state see Help information.)

Target nucleus: Atomic number: 92, Mass number: 234  
 Fissioning nucleus: Atomic number: 92, Mass number: 235

Induced fission with E\* distribution from file Espectrum.in  
 Spontaneous/CN fission  
 Neutron-induced fission

Neutron energy: 2.0 MeV

Shell effect at symmetry: 0.3 MeV

Enhancement factor: [ ]

Calculate only first-chance fission  
 Uncertainties and covariances from perturbed parameters  
 Record perturbed results (only for special use)  No plot  
 Use locally adjusted model parameters

Start calculation Clear Exit GEF

```

C:\GEF\GEF 2014\GEF.exe
Fission barrier of CN (Z= 92, A= 235):
Macrosc. barrier = 4.45 MeU
Inner saddle = 5.95 MeU, outer saddle = 5.87 MeU
exp. Mass = -1783.863 MeU
Lynase = -1783.61 MeU
G.S.Shell effect (Moeiler) = -1.46 MeU, G.S.Shell effect (exp,TF) = -1.74 MeU
S_n(exp.) = 5.297607 MeU
CN: Z = 92, A = 235, E = 2 MeU

Please wait ... code is running.

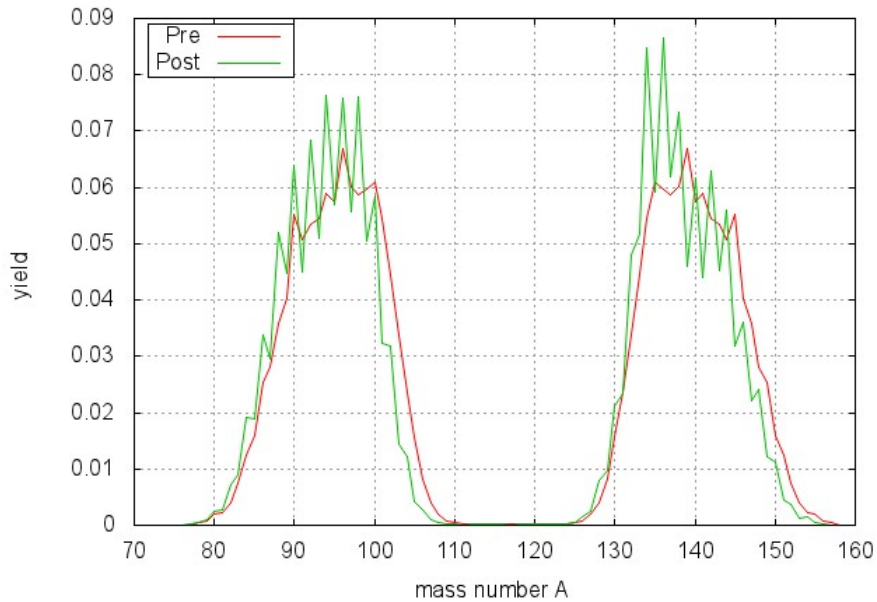
Calculation with nominal model parameters.
GEF 2 MeU
100000 events will be calculated.
Output is written to file
out\GEF.dat
  
```

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

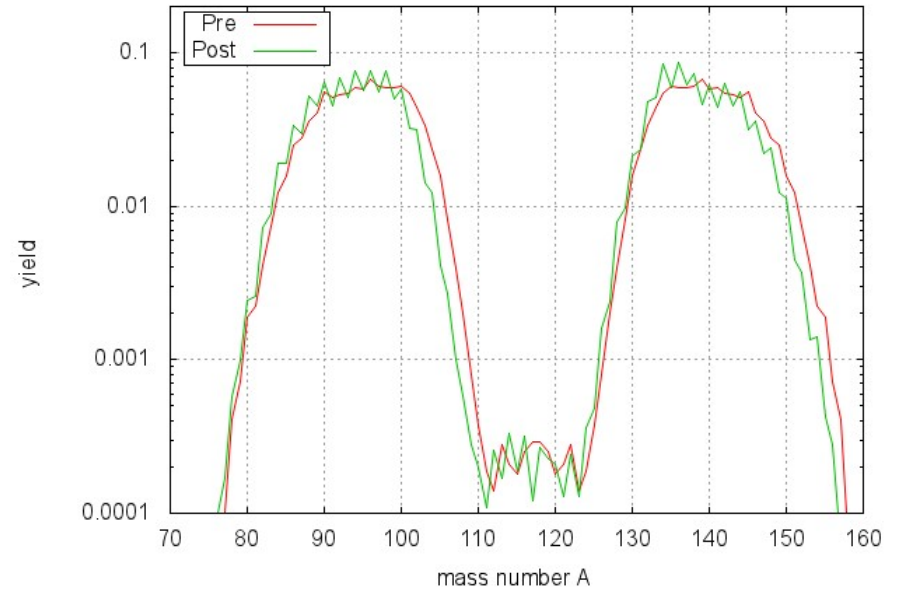


# TALYS-1.6 for $^{234}\text{U}(n,f)$

U-234(n,f) at 2 MeV from TALYS1.6

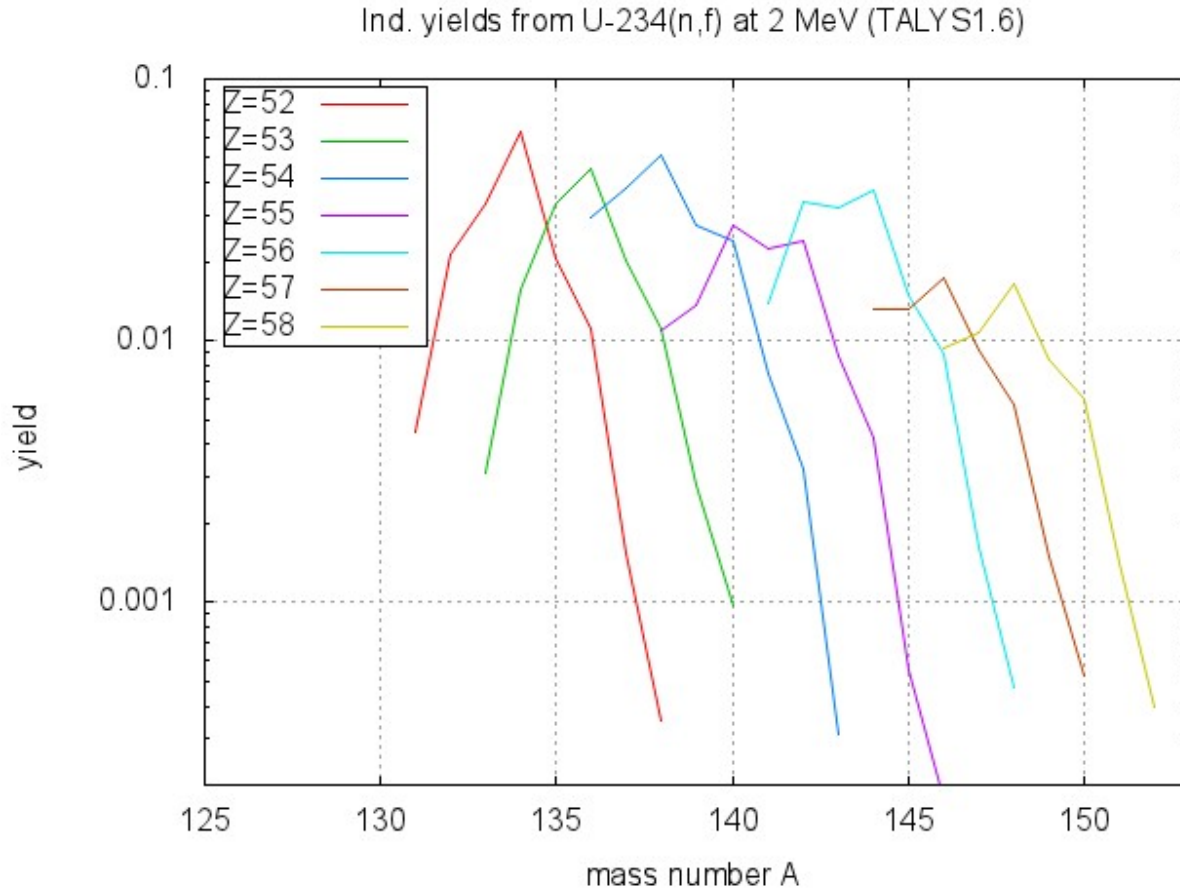


U-234(n,f) at 2 MeV from TALYS1.6





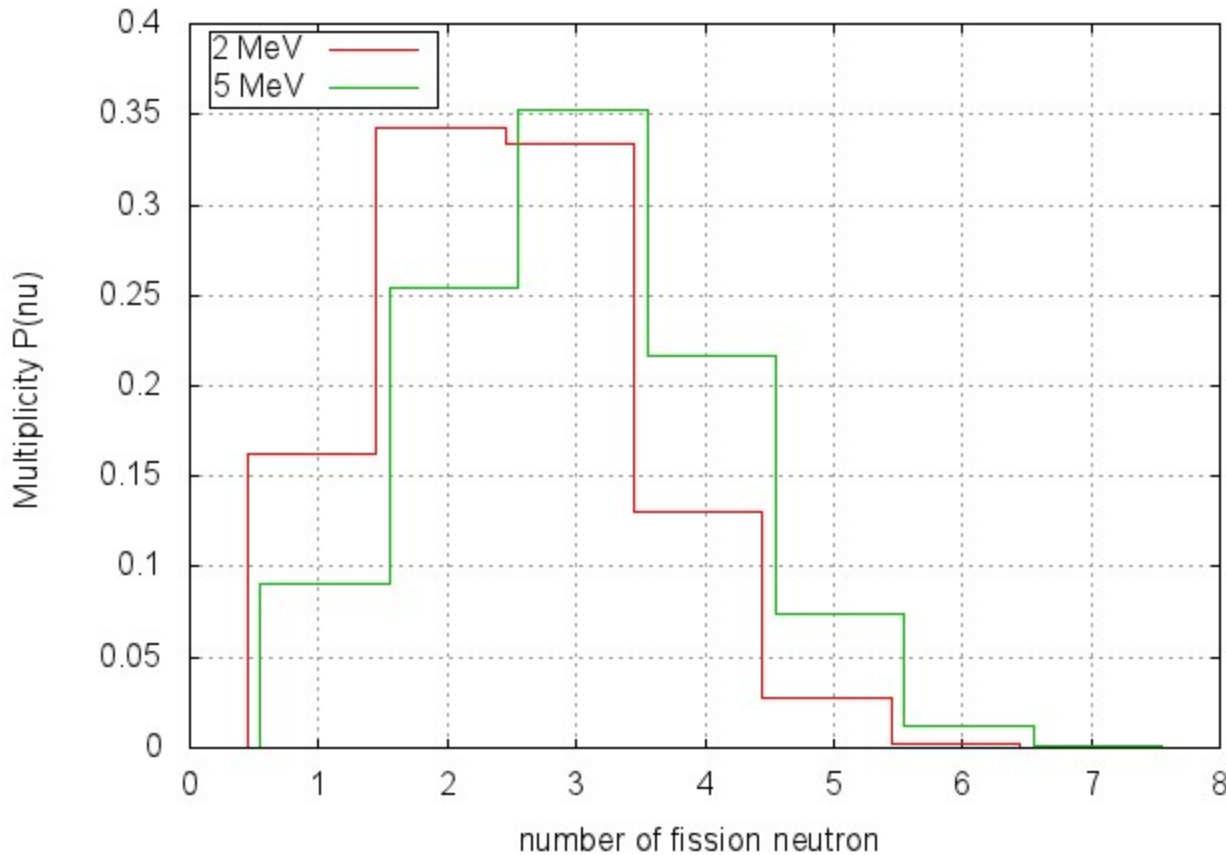
# Independent yields





# Neutron multiplicity

prompt neutron multiplicity from U-234(n,f) (TALYS1.6)



$$\bar{\nu} (2 \text{ MeV}) = 2.5250$$

JEF 3.1.2: 2.6176

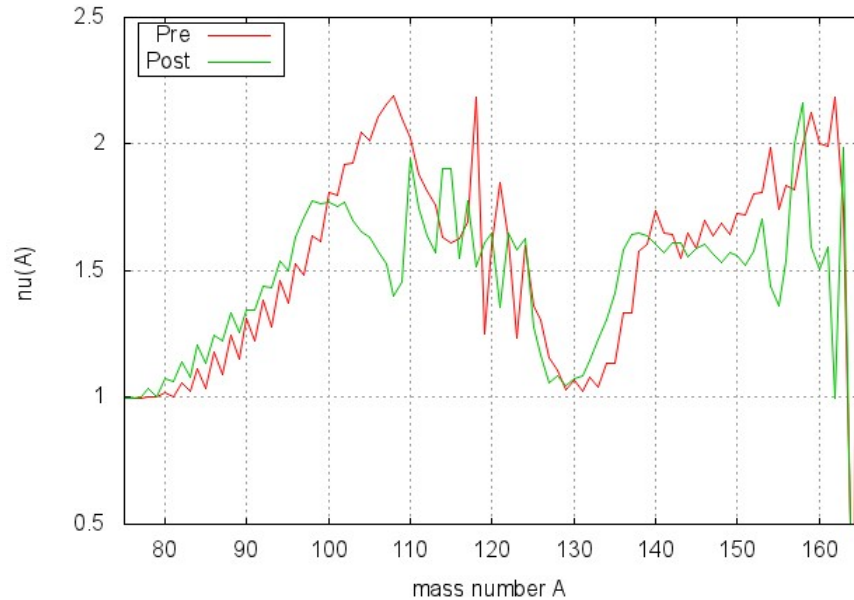
$$\bar{\nu} (5 \text{ MeV}) = 2.9714$$

JEF 3.1.2: 3.0275



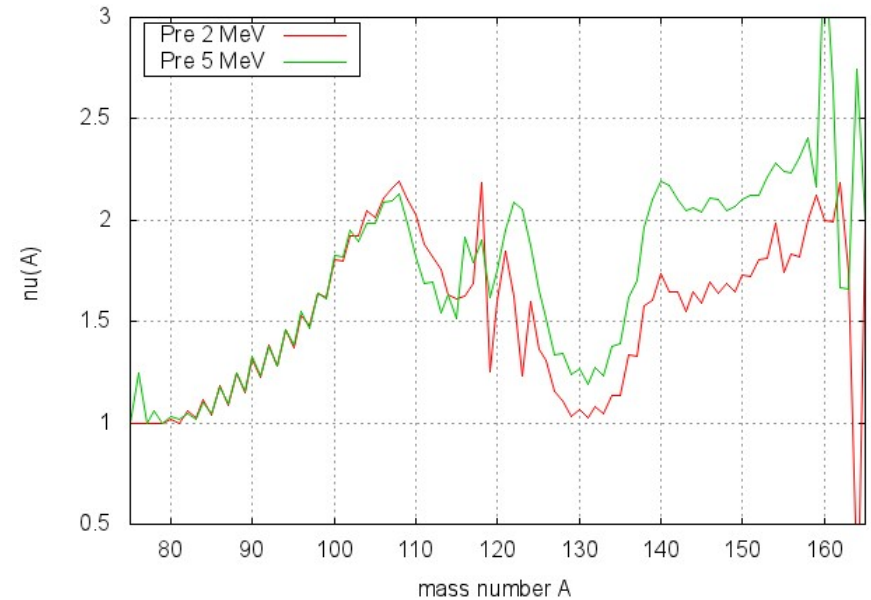
# TALYS-1.6 for $^{234}\text{U}(n,f)$

U-234(n,f) at 2 MeV from TALYS1.6



$\nu(A)$  pre- and post-neutron emission

U-234(n,f) at 2 and 5 MeV from TALYS1.6



$\nu(A)$  at 2 and 5 MeV (post)

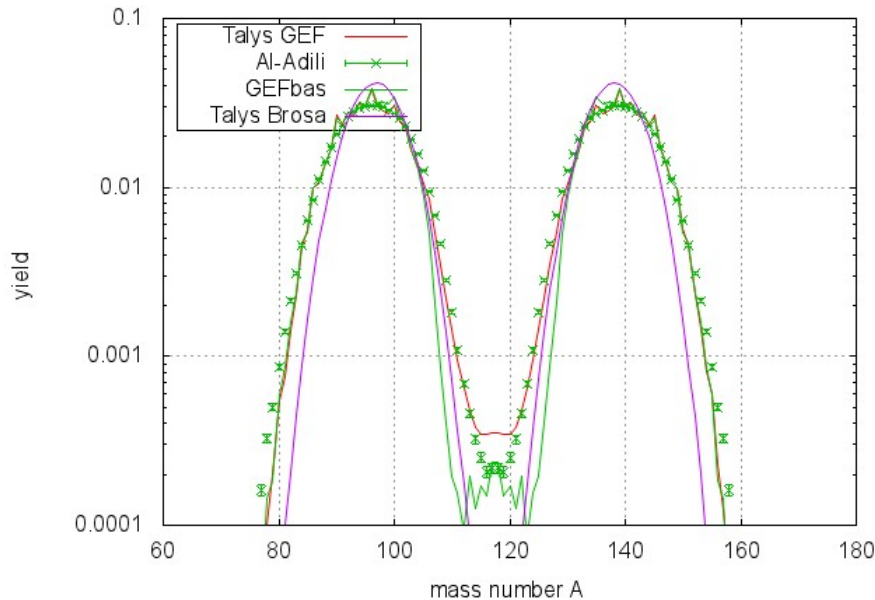
See Al-Adili et al., ND2013 proceedings,  
arXiv:1304.2278



# TALYS + GEF 2014/2.1

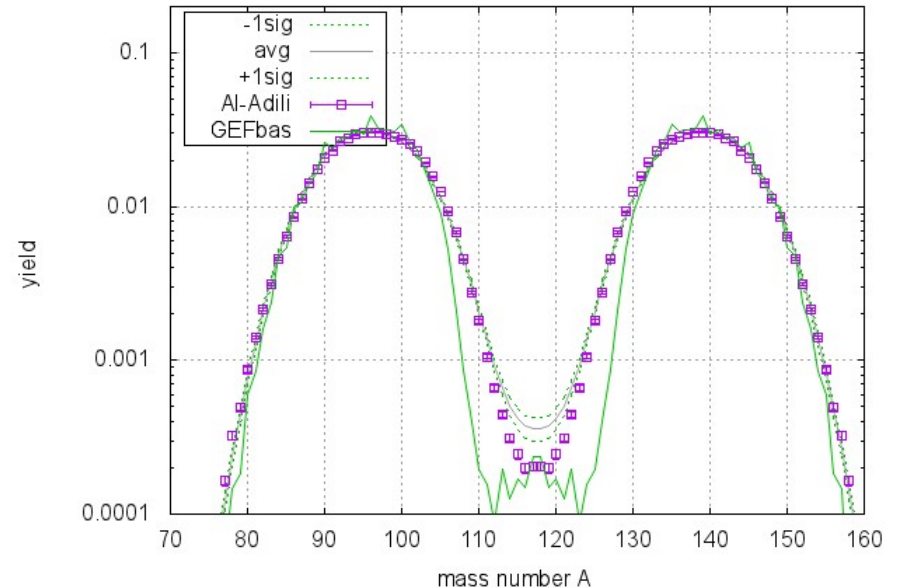
Use Fortran translation of the GEF fission code in TALYS 1.6:

FY - (n,f) - pre - TALYS+GEF2014



Comparison with GEF (Basic) and Brosa model in Talys

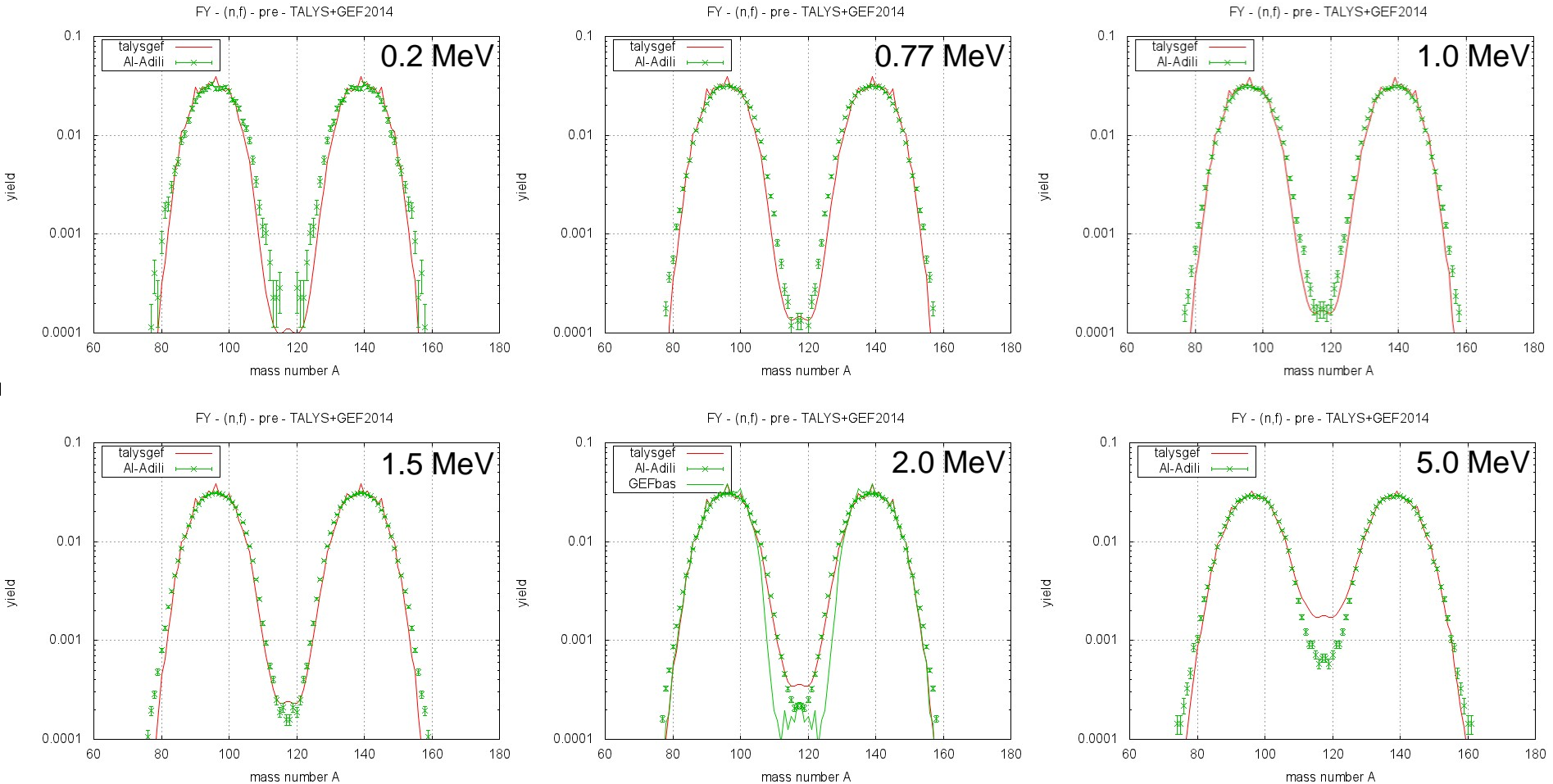
U-234(n,f) at 2 MeV (pre)



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



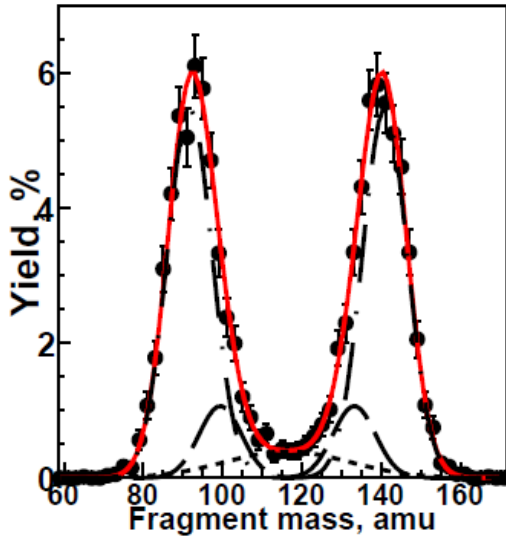
# TALYS+GEF2014 for $^{234}\text{U}(n,f)$



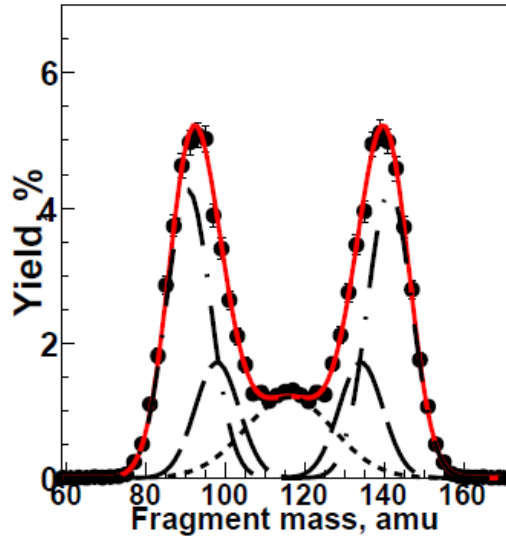


# $^{232}\text{Th}(n,f)$

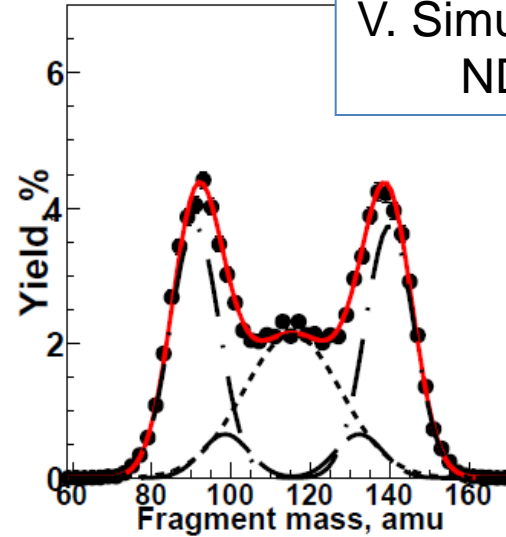
$^{232}\text{Th}(n,f)$ ,  $E_n = 9-11$  MeV



$^{232}\text{Th}(n,f)$ ,  $E_n = 14-19$  MeV

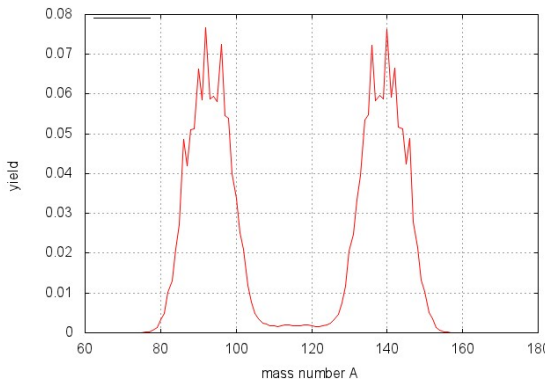


$^{232}\text{Th}(n,f)$ ,  $E_n = 26-40$  MeV

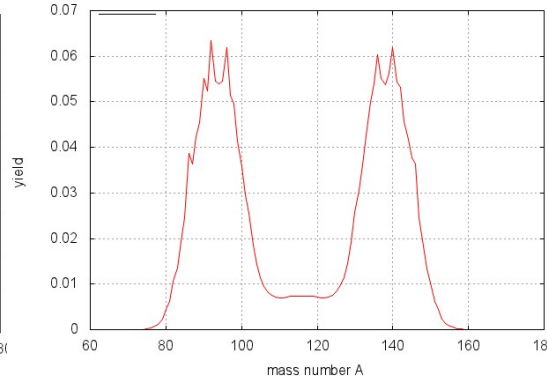


V. Simutkin et al.,  
ND2013

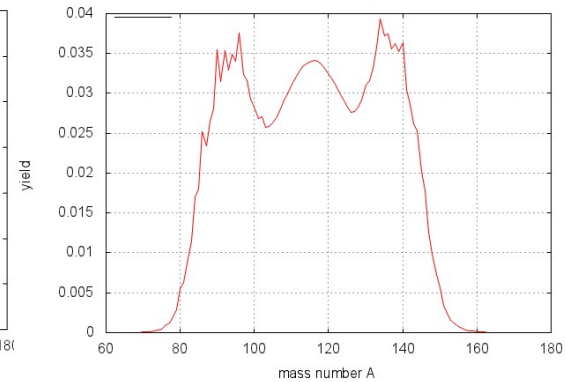
$^{232}\text{Th}(n,f)$  at 10 MeV - pre - TALYS+GEF2014



$^{232}\text{Th}(n,f)$  at 15 MeV - pre - TALYS+GEF2014



$^{232}\text{Th}(n,f)$  at 33 MeV - pre - TALYS+GEF2014

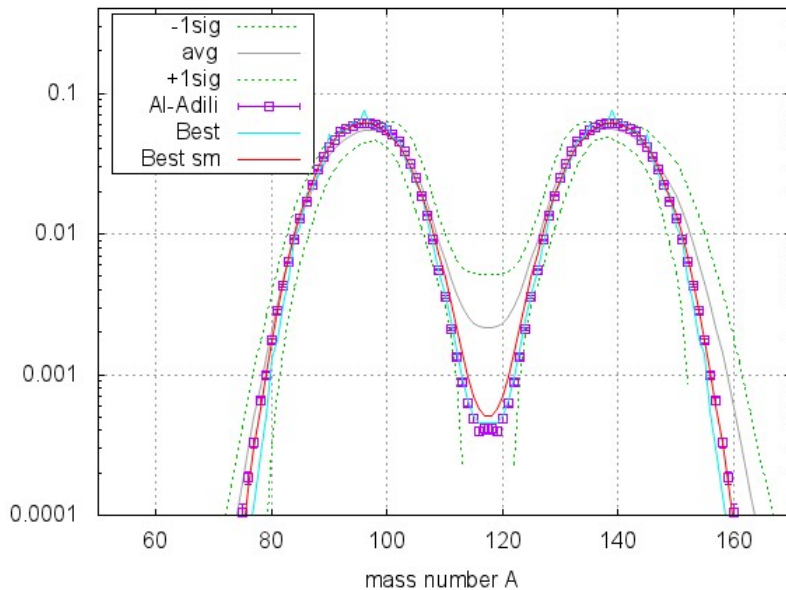




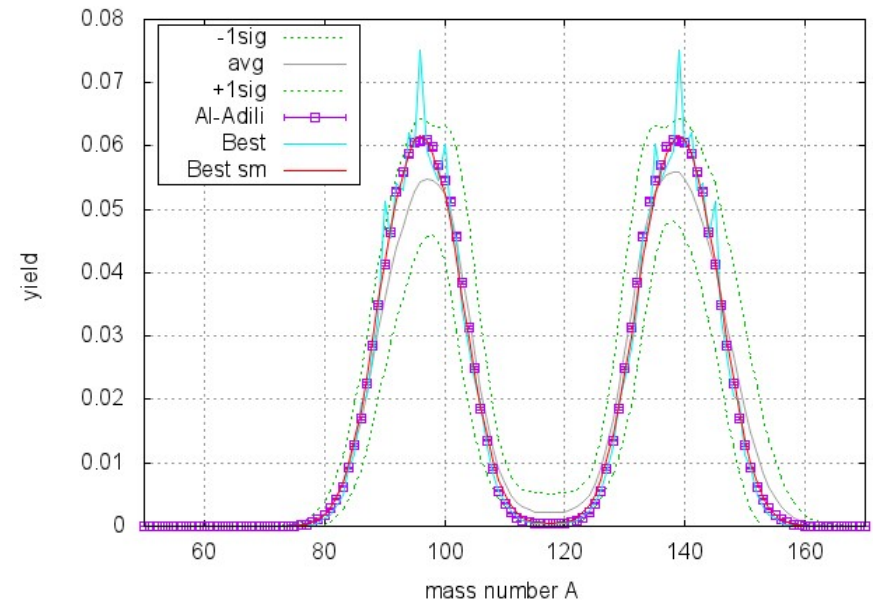
# Try randomizing parameters ...

500 TALYS+GEFSUB runs with randomization of 18 GEF parameters  
(10 times the uncertainties as given in GEF report from April 2014)

U-234(n,f) at 2 MeV (pre)



U-234(n,f) at 2 MeV (pre)

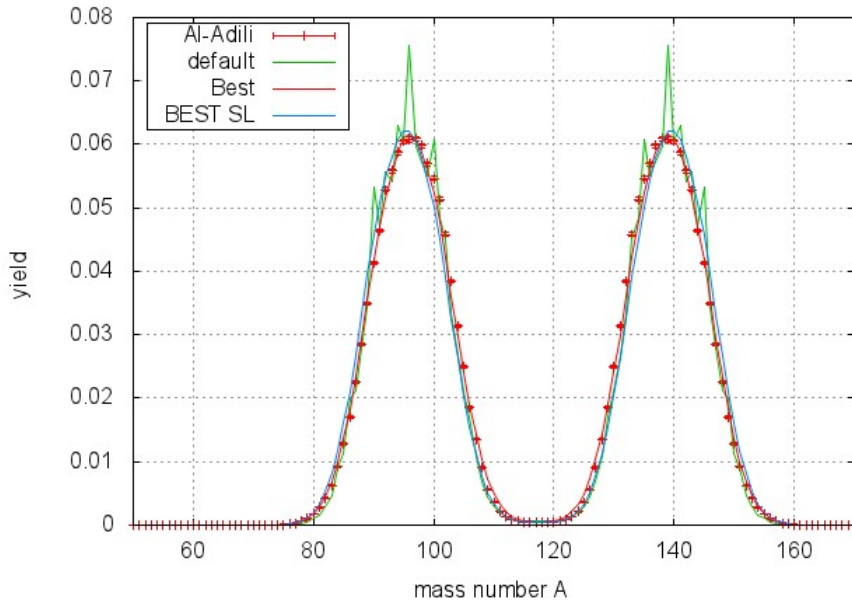


red curve: best TALYS+GEF run; adjusted to exp. resolution (4.5 AMU)

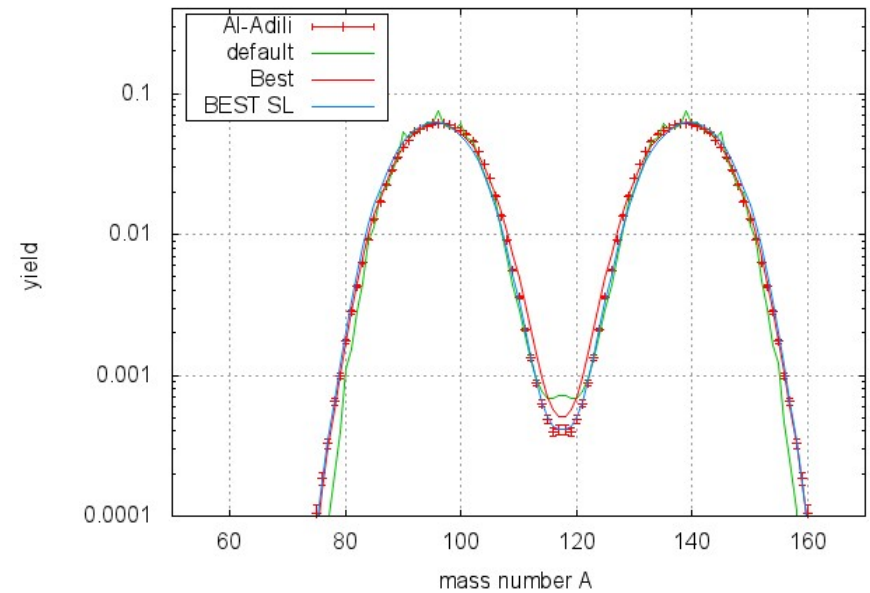


# TALYS+GEF2014: best fits in sym. region

U-234(n,f) at 2 MeV (pre)

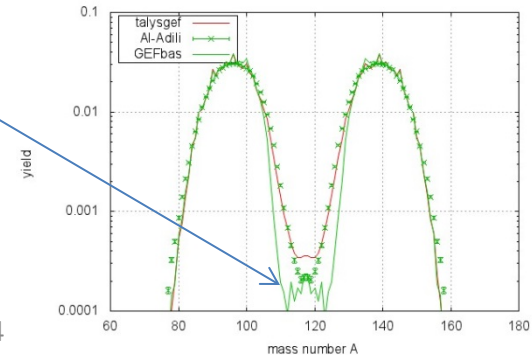


U-234(n,f) at 2 MeV (pre)



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

FY - (n,f) - pre - TALYS+GEF2014





# 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,  $\bar{\nu}$ .
  - 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



# 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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