DE LA RECHERCHE À L'INDUSTRIE

www.cea.fr

The TALYS code

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CEA, DAM, DIF

Content

- Introduction
- General features about the code
- Models implemented in TALYS
- Few example of results obtained with TALYS
- What remains to be done ?

INTRODUCTION

Why do we need nuclear data ?

Nuclear data needed for

Understanding basic reaction mechanism between particles and nuclei

Astrophysical applications (Age of the Galaxy, element abundances …)

Existing or future nuclear reactor simulations

Medical applications, oil well logging, waste transmutation, fusion, …

But

Finite number of experimental data (price, safety or counting rates)

Complete measurements restricted to low energies (< 1 MeV)
to scarce nuclei

→ **Predictive & Robust Nuclear models (codes) are essential**

Situation in 1998 !

ALICE – LLNL – 1974 – Blann

(Mc-)GNASH – LANL – 1977 – Young, Arthur & Chadwick

TNG – ORNL – 1980 – Fu

STAPRE – Univ. Vienna – 1980 – Uhl

UNF,MEND – CIAE, Nanking Univ. – 1985 – Cai, Zhang

EXIFON – Univ. Dresden – 1989 – Kalka

EMPIRE – ENEA/IAEA/BNL – 1980 – Herman

TALYS – NRG/CEA – 1998 – Koning, Hilaire & Duijvestijn

Modern computers (i.e. speed and memory) available when the code conception was started

GNASH Input file before 1998

```
PU238 + n fission calculation -
input with wrong parameters
   1   0   0   3   1  01   0   0
   0   0   0   0   0 108   1   1   0   0   0   0   1   0   1   0   0   0   0
  14   3   3   1   0   1   1   2   1   2   0   1   0   0   2   0   6   1
 300   0
   2   0   4   5     0.00     0.00
 1.        94238.        0.010     0.000   0.04408     2.000     1.000
2.000
 0.0888     0.0      0.0
 80
 0.001       0.002     0.004     0.006     0.008       0.01      0.02        0.03
 0.04        0.05      0.06      0.07      0.08        0.09      0.1         0.2
 0.3         0.40      0.50      0.60      0.70        0.80      0.90        1.0
 1.1         1.20      1.30      1.40      1.50        1.60      1.70        1.80
 1.9         2.00      2.1       2.20      2.30        2.40      2.50        2.60
 2.7         2.80      2.9       3.00       3.50        4.       4.5         5.
 5.5         6.00      6.5       7.00       7.50        8.       8.5         9.
 10.         11.       12.       13.       14.         15.       16.        17.
 18.         19.       20.       21.       22.         23.       24.        25.
 25.5       26.       27.       28.       29.         30.       31.        32.
 94239.    8.            0.            0.          +0.1245
 0.        0.        0.       28.        0.2590   25.        0.        0.
 0.        0.        0.        0.        0.        0.
 1.        0.        0.       24.        0.2642   17.        0.        0.
-0.5590    0.8610    5.9000    0.        0.        0.
 1001.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 1002.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 1003.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 2003.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 2004.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 99.       0.        0.        0.        0.000     0.        0.        0.
 0.        0.        0.        0.        0.        0.
 94238.    8.            1.            2.          -0.
 0.        0.        0.       24.        1.8642   17.        0.        0.
-1.2590    0.8610    4.3000    0.        0.        0.
 1.        0.        0.       19.        0.7735   18.        0.        0.
-1.7700    0.5740    0.        0.        0.        0.
 1001.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 1002.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 1003.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 2003.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 2004.     0.        0.        0.        0.        0.        0.        0.
 0.        0.        0.        0.        0.        0.
 99.       0.        0.        0.        0.000     0.        0.        0.
```

GENERAL FEATURES ABOUT

THE CODE

IDEAS BEHIND TALYS CONCEPTION

- TALYS mantra : " First Completeness then Quality"

No NaNs
No Crash
Warnings to identify malfunctions
Default « simple » models which will then be improved (anticipation)
All ouput channels smoothly described

- Transparent programming

No unnecessary assumption
No equation simplification (one can recognize a general expression)
Many comments
No implicit definition of variables
The variable are defined following the order of appearance in subroutines

WHAT TALYS DOES !

- Simulates a nuclear reaction

  projectiles : n,p,d,t,^{3}he, ^{4}he and gamma
  targets : $3 \leq Z \leq 110$ or $5 \leq A \leq 339$ (either isotopic or natural)

- Incident projectile energy from a few keV up to 200 MeV
  code works up to1 Gev but physics ??

- TALYS can be used :

  . In depth single reaction analysis

  . Global nuclear reaction network calculation (eg astrophysics)

  . Within a more global code system (reactor physics)

  . Without reaction calculation (only structure data provided)

- TALYS is still under development (improvement)

TECHNICAL DETAILS

- Fortran 77

- ≈ 80000 lines (+ 20000 lines of ECIS)

- Modern programming
  - modular (270 subroutines)
  - Explicit variable names and many comments (30% of total number of lines)
  - Transparent programming (few exceptions)

- Flexible use and extensive validation
  - Flexibility : default ⇒ 4 line idiot proof input (element, mass, projectile, energy)
    adjustment ⇒ 300 keywords
  - Random input generation to check stability
  - Drip-line to drip-line calculations help removing bugs

- >500 pages manual

- Compiled and tested with several compilers and OS

TYPICAL CALCULATION TIMES

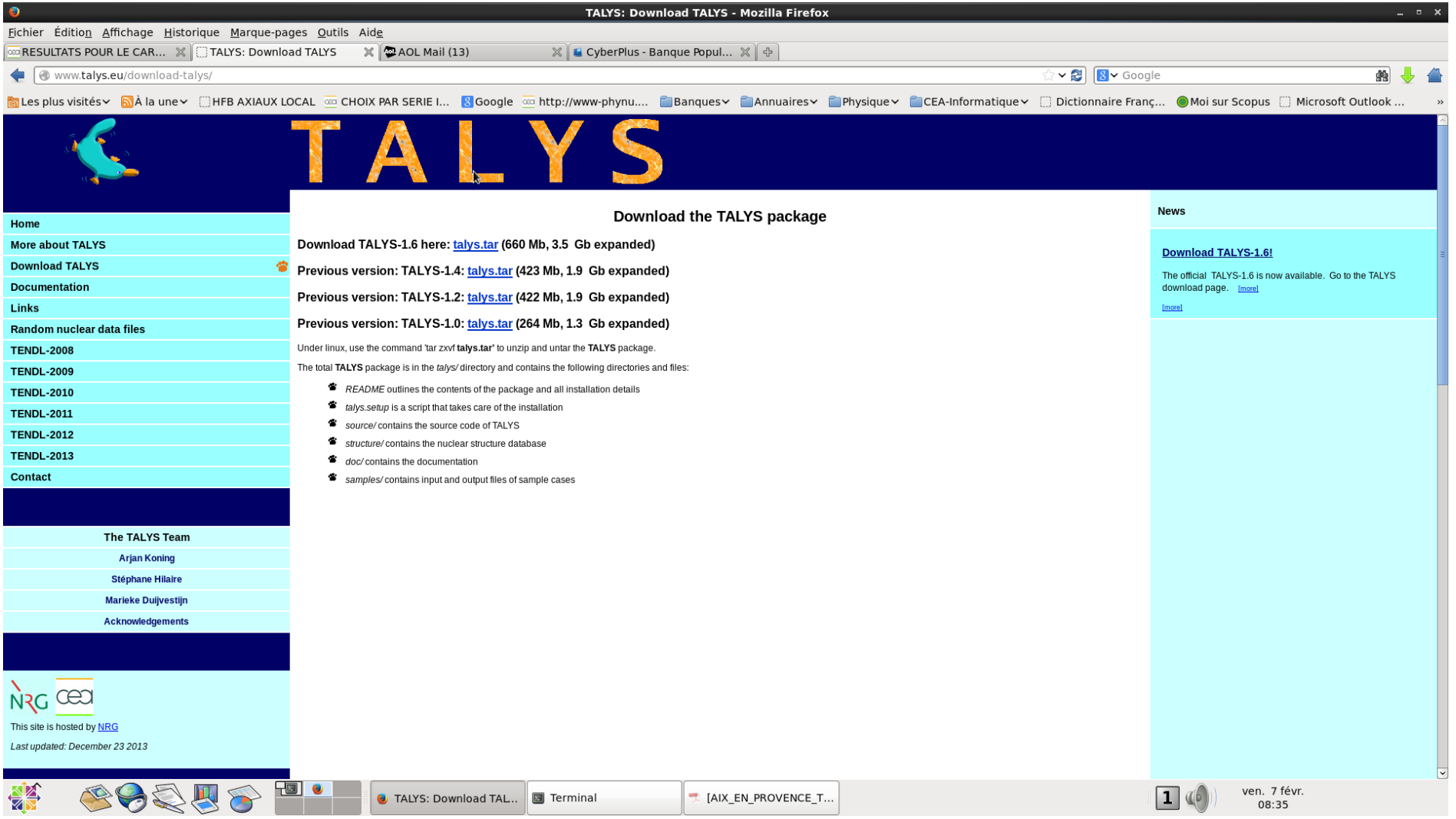
Numbers based on a single Intel Xeon X5472 3.0 GhZ processor

Time needed to get all cross sections, level densities, spectra, angular distributions. gamma production etc.:

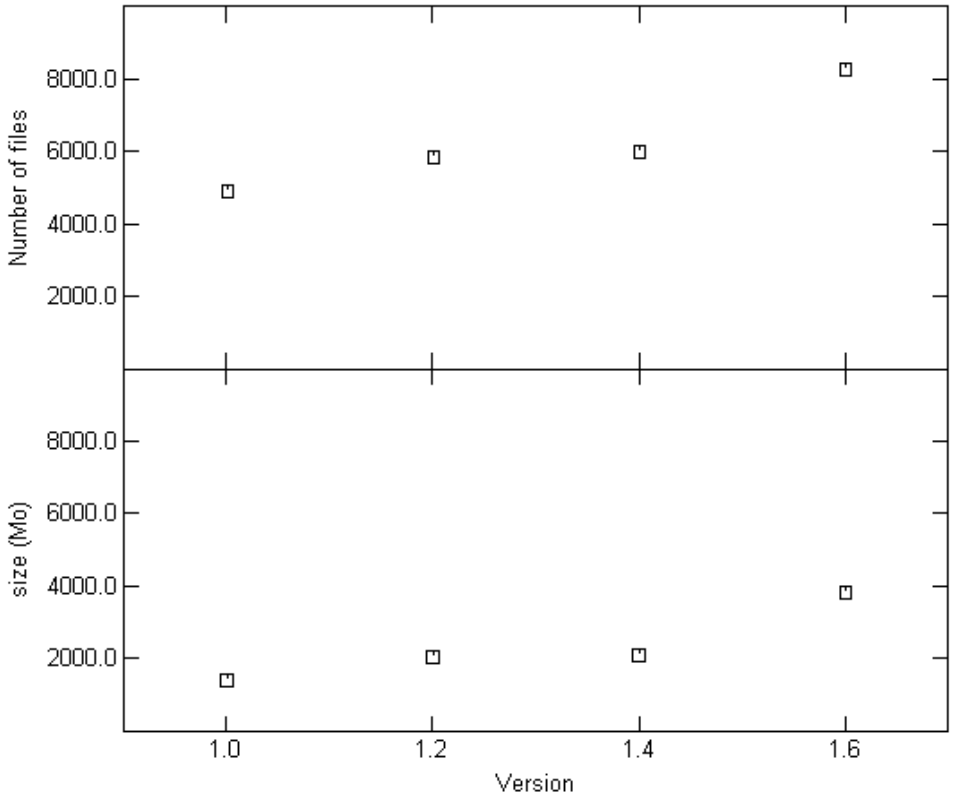
- **14 MeV neutron on non-deformed target: 3 sec.**
- **60 incident energies between 0 and 20 MeV:1 min. (Al-27)**
  4 min. (Pb-208)
  10 min. (U-238)
- **100 incident energies between 0 and 200 MeV:20 min. (Al-27)**
  3-100 hours (U-238) depending on OMP
- **60 incident energies between 0 and 20 MeV for all 2430 nuclides, stable or with t> 1 sec: about 200 hours**
- **To obtain credible Monte Carlo based covariance data: multiply the above numbers by 50-500.**

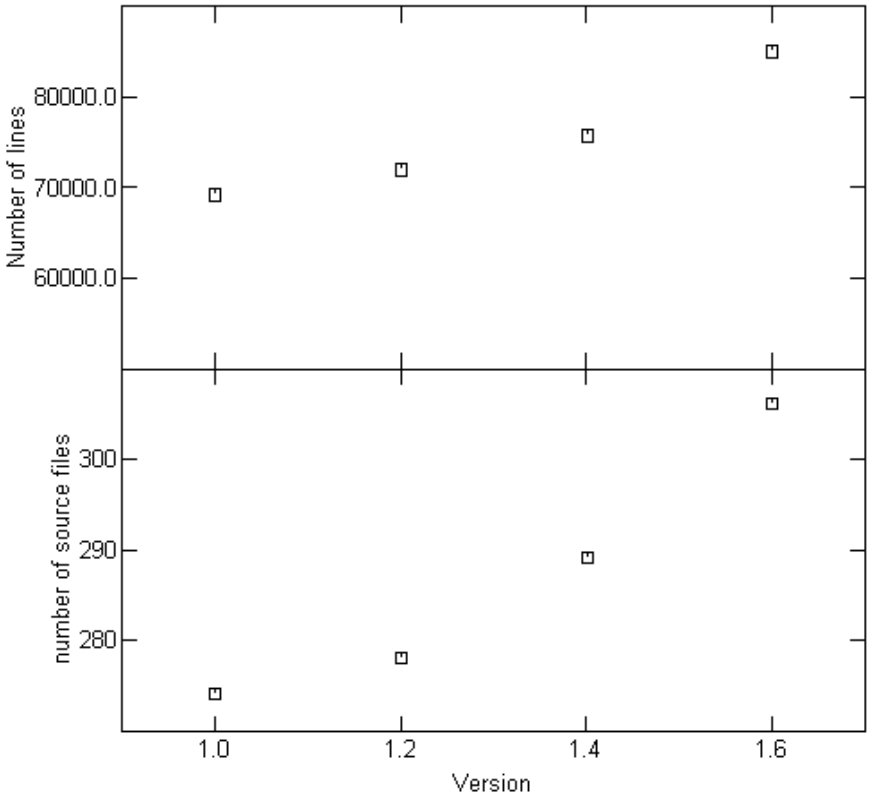
TALYS VERSIONS ONLINE

http://www.talys.eu



TALYS STATISTICS

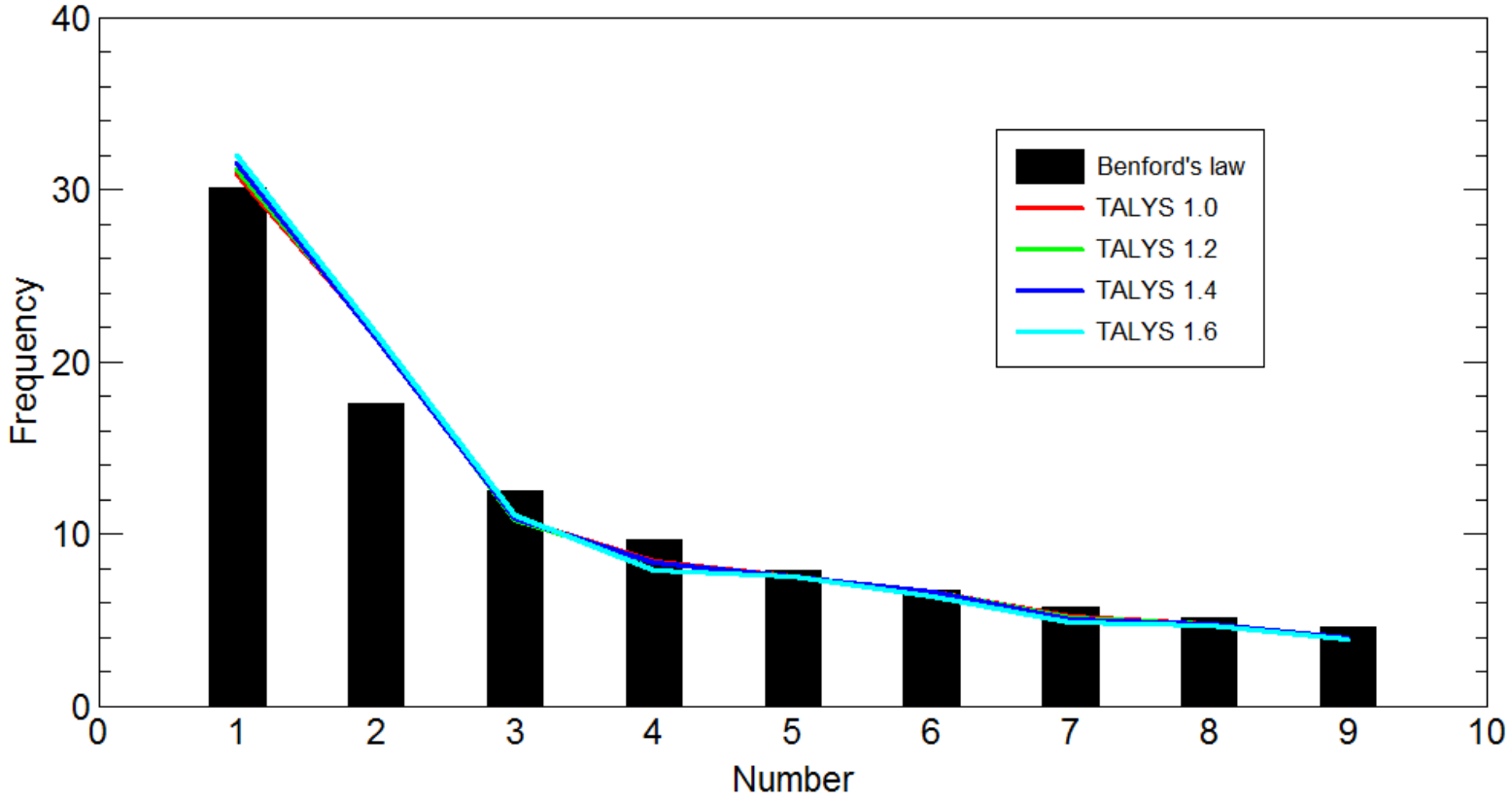




Inclusion of ph lds

Inclusion of 1p1h lds function of (J,π)

TALYS STATISTICS



TALYS obeys the Benford's law : no intentional scientific fraud

TALYS VERSIONS (HISTORY)

TALYS 1.0 (ND 2007)

TALYS 1.2 (End of 2010)

- **new keywords (mainly to improve fitting possibilities)**
- **bugs corrected to solve crashes or unphysical results**
- **inclusion of ph level densities**
- **inclusion of Skm-HFB structure information (def., masses, γ strengths)**
- **inclusion of D1M**

TALYS 1.4 (End of 2012)

- **new keywords (mainly to improve fitting possibilities)**
- **bugs corrected to solve unphysical results or crashes**
- **new alpha and deuteron OMP**
- **URR extension**

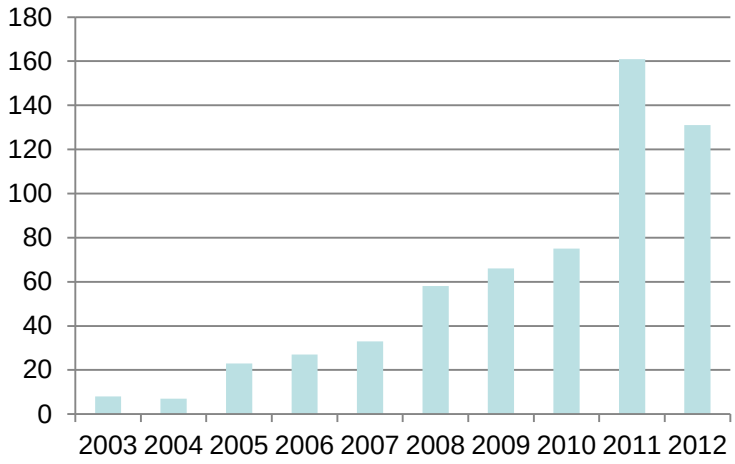
TALYS 1.6 (End of 2013)

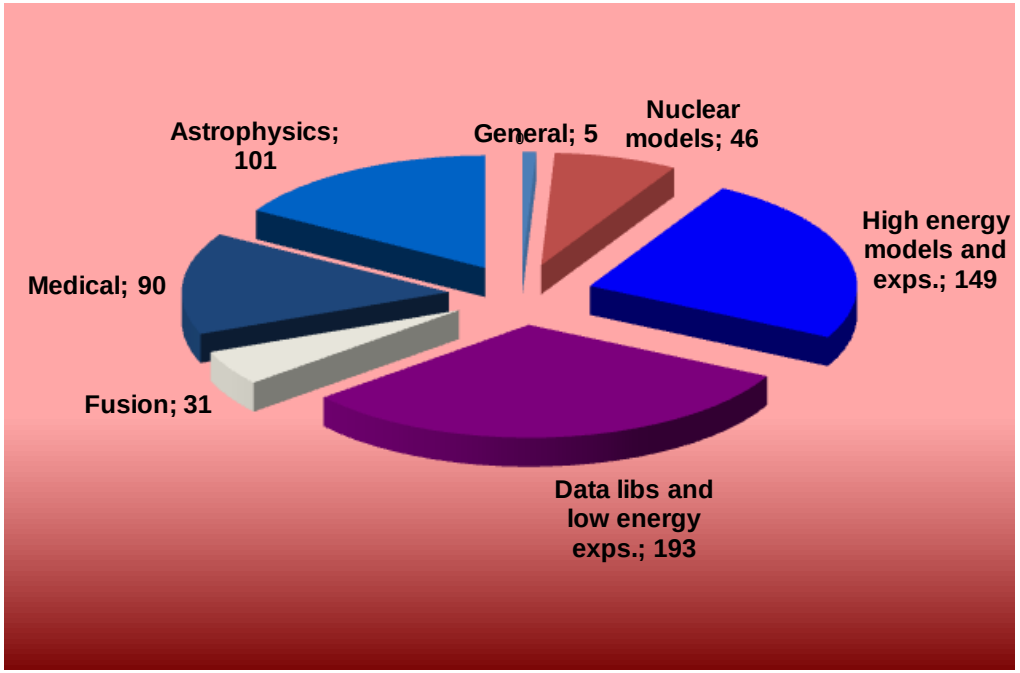
- **bugs corrected to solve unphysical results or crashes**
- **non-equidistant excitation energy binning possible (extension to energies > 200 MeV)**
- **direct and semi-direct capture added**
- **new microscopic lds from D1M**
- **medical isotope production implemented**
- **coupling to GEF done**

TALYS USERS and PUBLICATIONS

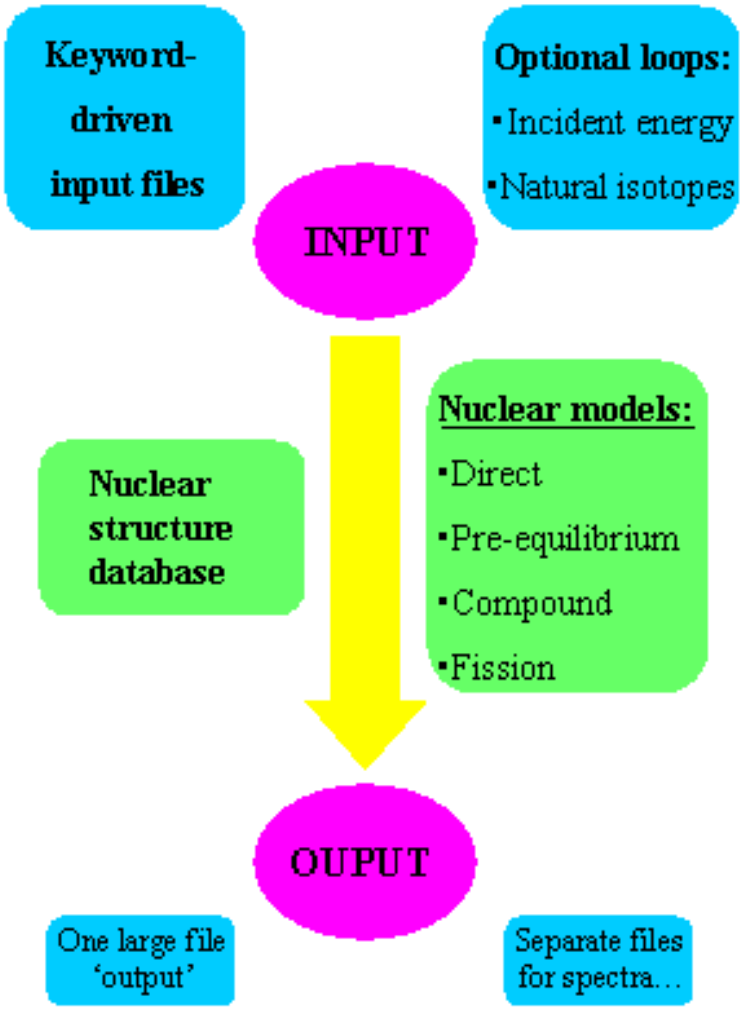
- User feedback via talys mailing list : info@talys.eu to be added to mailing list
  : talys-l@nrg.eu to inform mailing list

PUBLICATIONS





TALYS SCHEME



WHAT TALYS YIELDS

Cross sections :

total, reaction, elastic (shape & compound), non-elastic, inelastic (discrete levels & total)
total particle production
all exclusive reactions (n,nd2a)
all exclusive isomer production
all exclusive discrete and continuum γ-ray production

Spectra :

elastic and inelastic angular distribution or energy spectra
all exclusive double-differential spectra
total particle production spectra
compound and pre-equilibrium spectra per reaction stage.

Fission observables :

cross section (total, per chance)
fission fragment mass and isotopic yields

Miscellaneous :

recoil cross sections and ddx
particle multiplicities
s and p wave functions and potential scattering radius r'
nuclear structure only (levels, Q, ld tables, …)
specific pre-equilibrium output (ph lds, decay widths …)
astrophysical reaction rates

TALYS VALIDATION

- Validation with the drip code

Drip (not released) performs drip line to drip line calculation

⇒ No Crash

⇒ Checking results smoothness

- Validation with the monkey code

Monkey (not released) creates random input for TALYS

⇒ No Crash

⇒ Checking robustness with respect to crazy input (within allowed ranges) values

- Validation of level density models with the kh05 code

kh05 (not released) automatically adjust level densities to data

⇒ global and local level density models

TALYS has then be used to perform extensive comparisons between theoretical and experimental cross sections for (n,γ), (n,2n), (n,p), (n,d) and (n,α) with all possible ld models

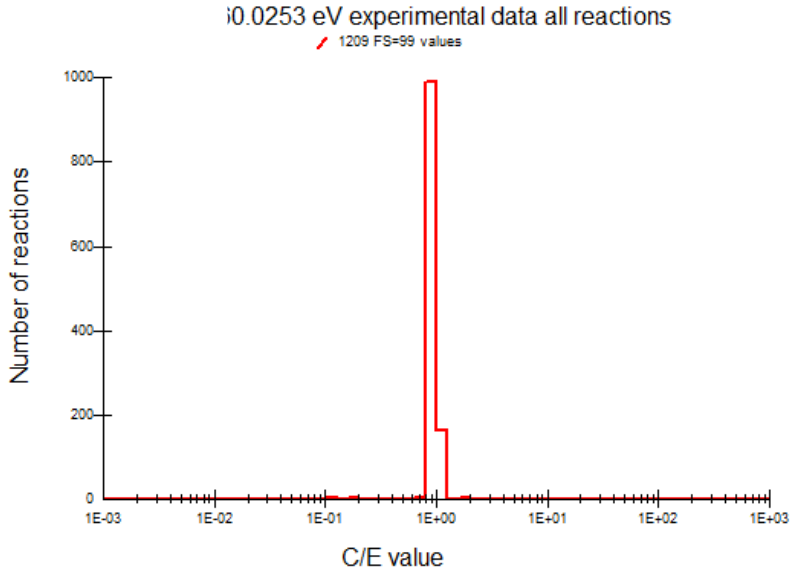
- Statistical analysis of cross sections - SACS (J. Kopecky)

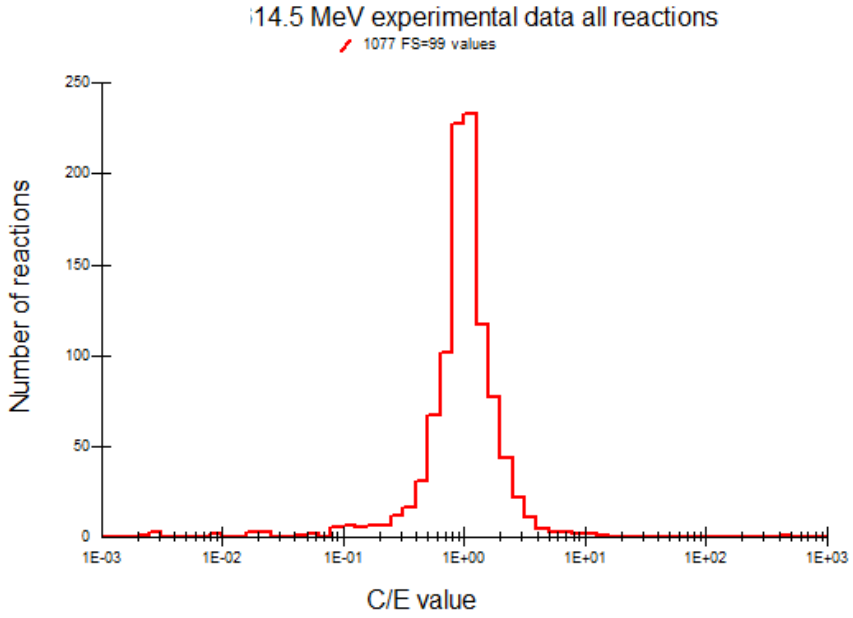
Extensive comparison of cross section with data from EXFOR

⇒ C/E values

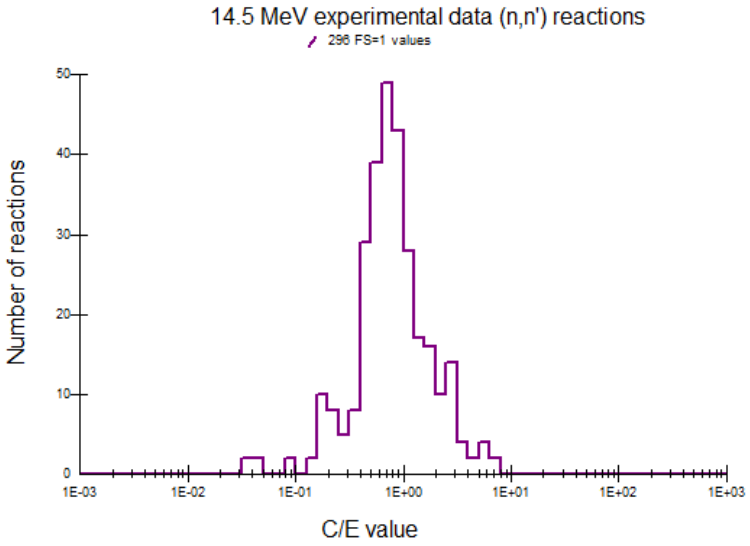
⇒ Shape analysis (maximum xs, energy of maximum, half width at maximum)

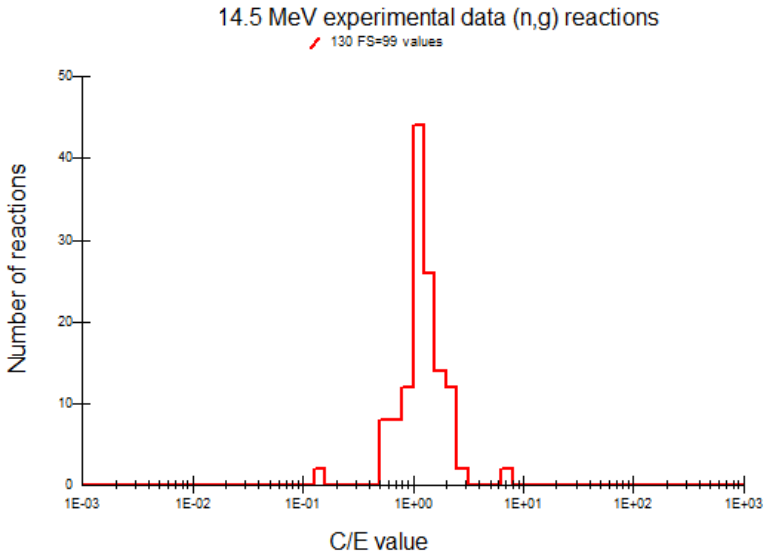
TALYS VALIDATION (SACS 1/3)

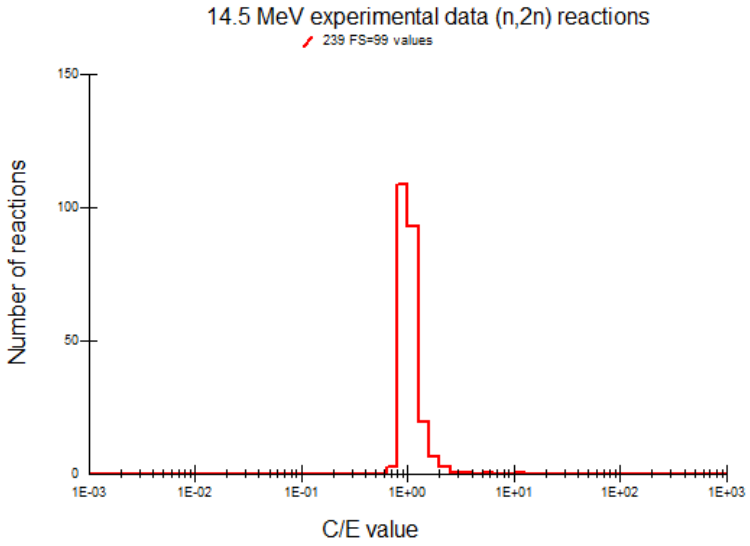


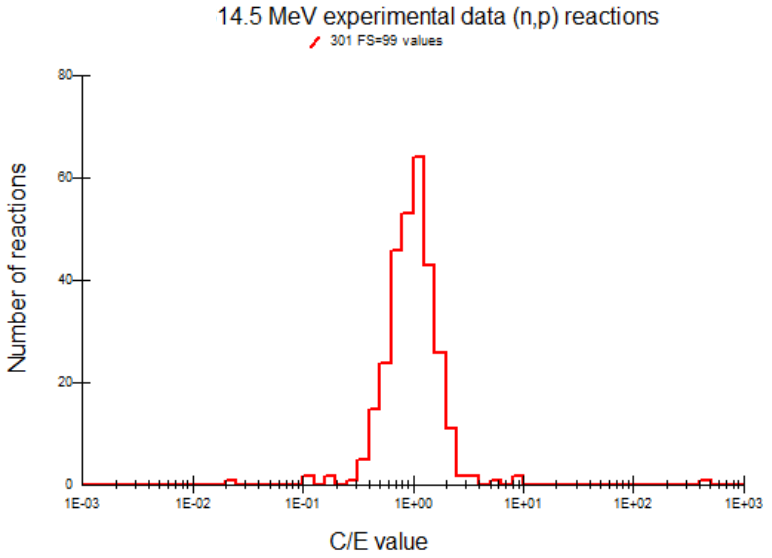


TALYS VALIDATION (SACS 2/3)

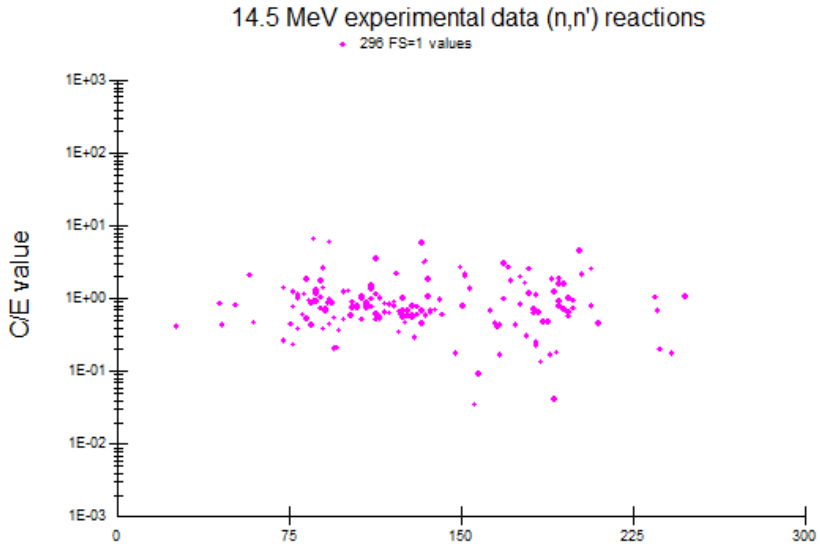


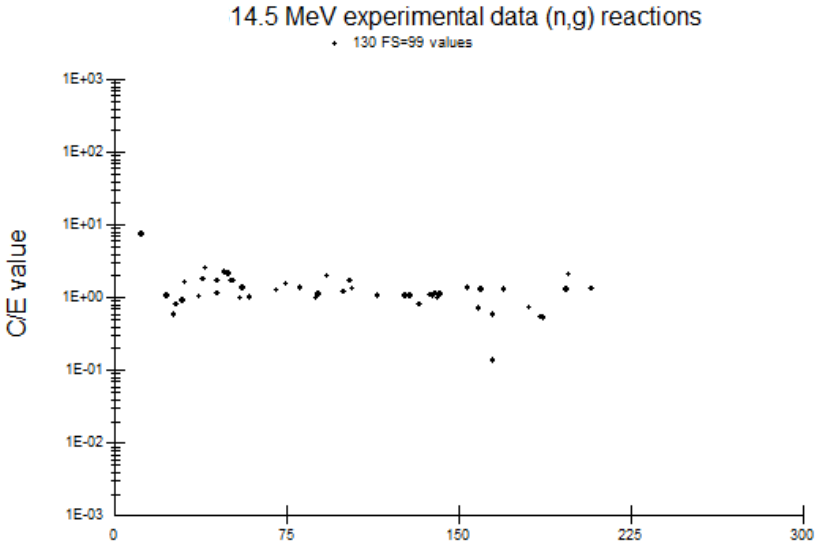


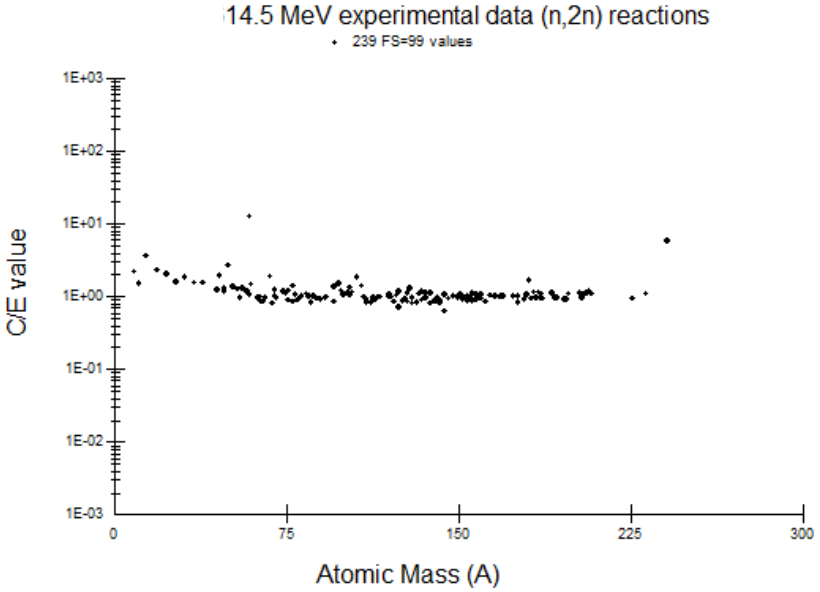


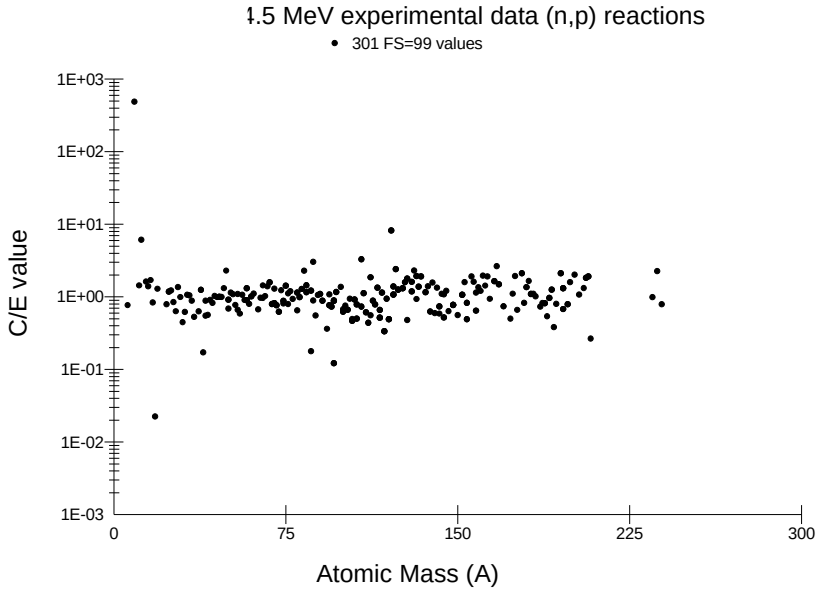


TALYS VALIDATION (SACS 3/3)









MODELS IMPLEMENTED

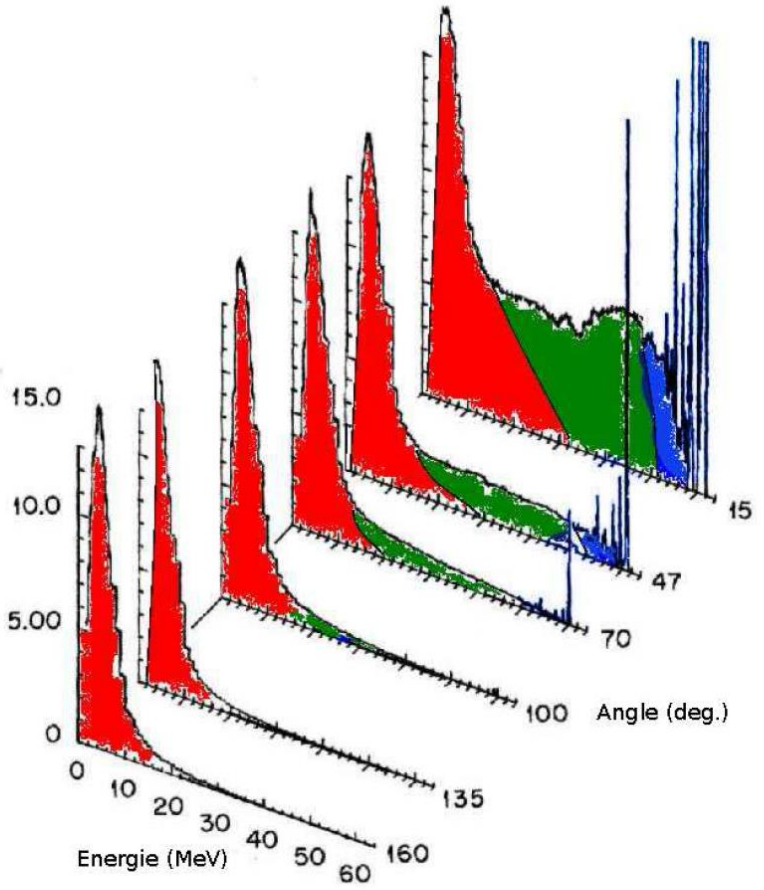
IN TALYS

TYPICAL DDXS and MODELS (non fissile)

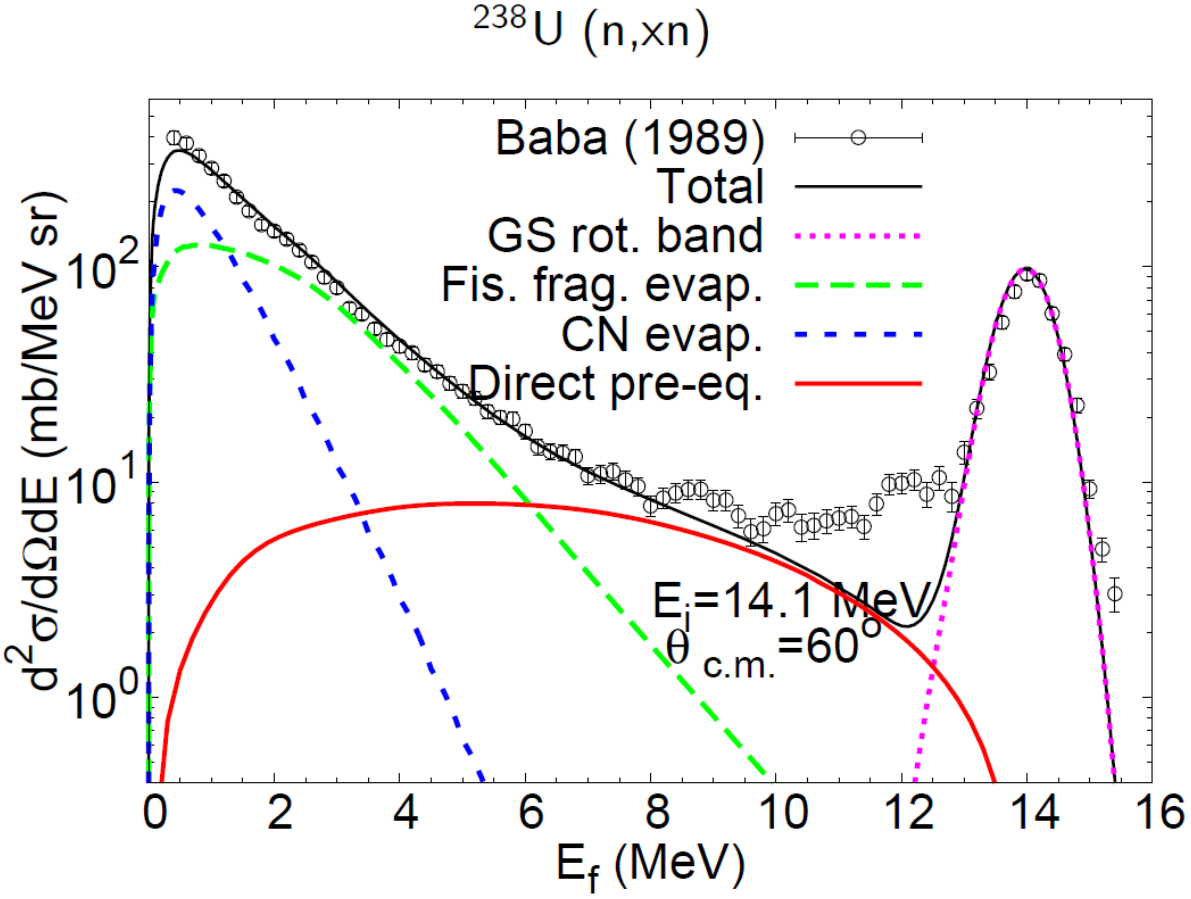
Compound decay

Pre-equilibrium component

Direct component



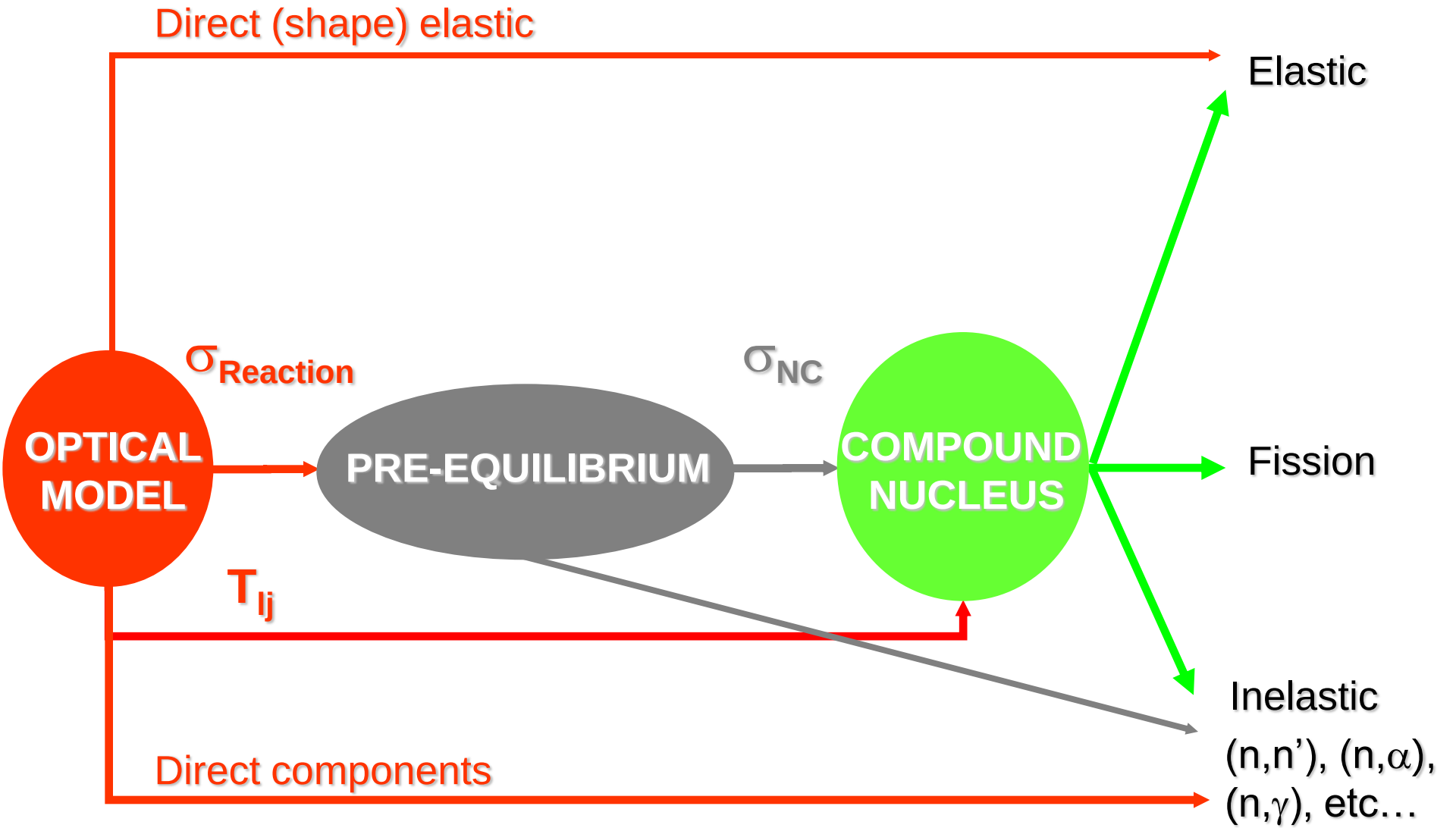
TYPICAL DDXS and MODELS (fissile)



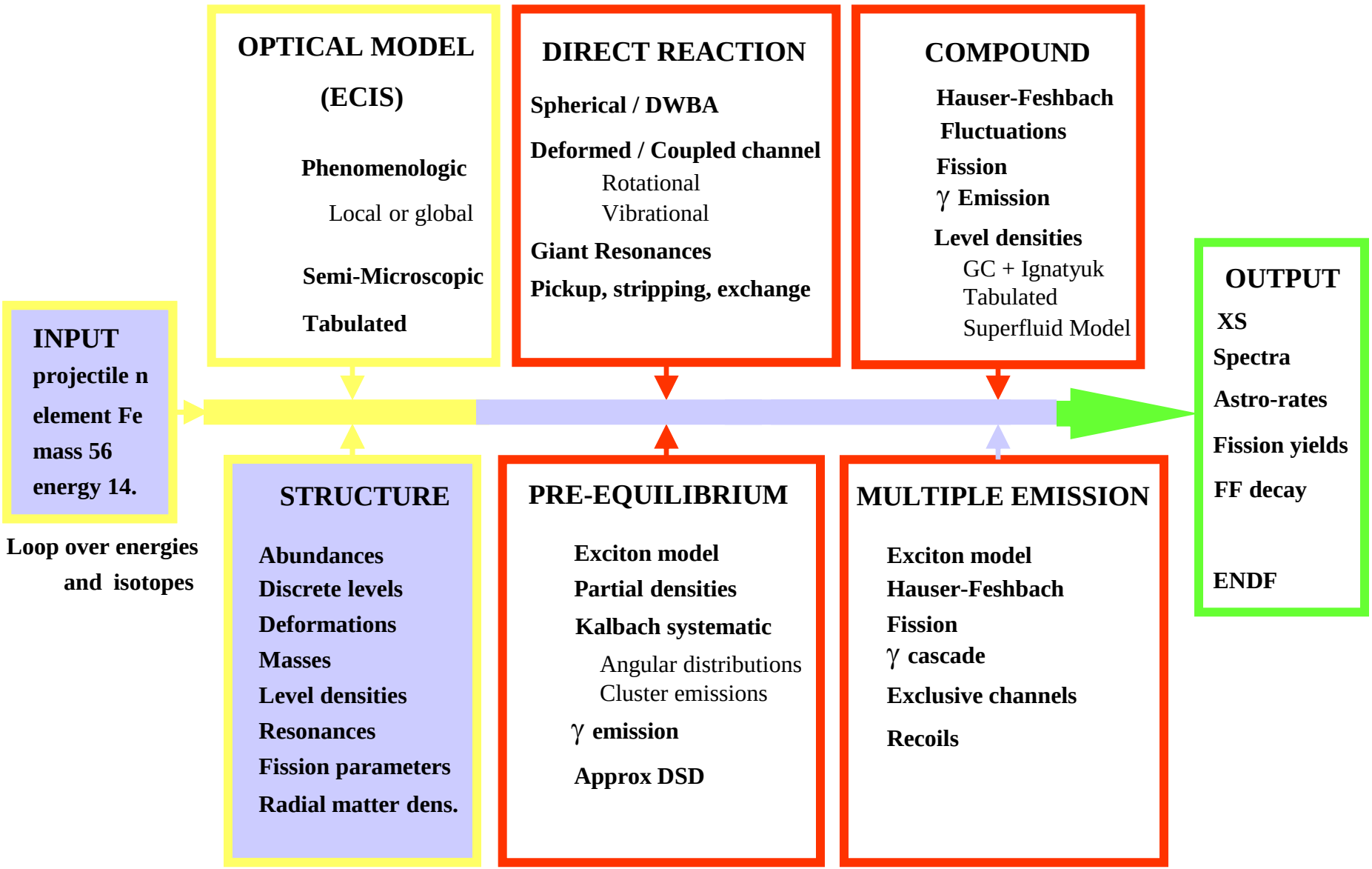
⇒ prompt fission neutron spectra required

⇒ something missing so far around 10-12 MeV (see M. Dupuis)

MODELS SEQUENCE



TALYS SCHEME (with more details)



OPTICAL MODELS

Optical model potential (OMP) calculations are performed with ECIS-2006

Neutrons/protons: Koning-Delaroche phenomenological spherical OMP (local / global)

Soukhovitskii deformed OMP for actinides

User-defined OMPs

Dispersive OMPs

Hartee-Fock-Bogolyubov based JLM OMPs

Simplified Watanabe folding approach for complex particles

DIRECT REACTIONS

Direct reaction calculations are performed with ECIS-2006

DWBA for (near) spherical nuclei

Coupled-channels for deformed nuclei

Symmetric rotational / Harmonic vibrational / Vibration-rotational / Asymmetric rotational

Weak-coupling model for odd nuclei

Giant resonances (Kalbach macroscopic phenomenological model)

COMPOUND REACTIONS

Hauser-Feshbach (Full spin coupling)

⇒ Width-fluctuation models (Moldauer / GOE triple integral / HRTW)

⇒ Blatt-Biedenharn formalism for angular distributions

Astrophysical reaction rates by Maxwellian folding of the cross sections

Initial excited nucleus with excitation energy population

⇒ Testing surrogate reactions

⇒ Coupling with other codes (ex GEF)

Multiple Hauser-Feshbach emission for any number of particles

LEVEL DENSITIES

Gilbert-Cameron model

Back-shifted Fermi gas model

Generalized Superfluid model

Ignatyuk damping of shell effects in the level density parameter

Rotational / vibrational effects

Microscopic level densities based on Hartree-Fock-Bogolyubov model
(non statistical spin and parity dependencies)

PRE-EQUILIBRIUM REACTIONS

Two-component exciton model

Photon exciton model (Akkermans and Gruppelaar)

Continuum stripping, pick-up, knock-out and stripping (Kalbach phenomenological model)

Angular distribution (Kalbach systematics)

Multiple pre-equilibrium emission for any number of particles

Microscopic ph state densities (not fully tested)

GAMMAS

Brink-Axel Lorentzian

Kopecky-Uhl Generalised Lorentzian

Microscopic HFB gamma-ray strength functions (table)

Photoabsorption cross sections: GDR + quasi-deuteron (Chadwick)

FISSION

Hill-Wheeler transmission coefficients

single / double / triple humped barriers

Class II (III) states

Experimental barrier parameters

Rotating-Liquid-Drop model

Rotating-Finite-Range model

Microscopic barrier parameters + WKB approximation of fission path

Fission fragment mass distributions (Multi-Model Random-Neck-Rupture model)

Fission fragment charge disitributions (scission-point model)

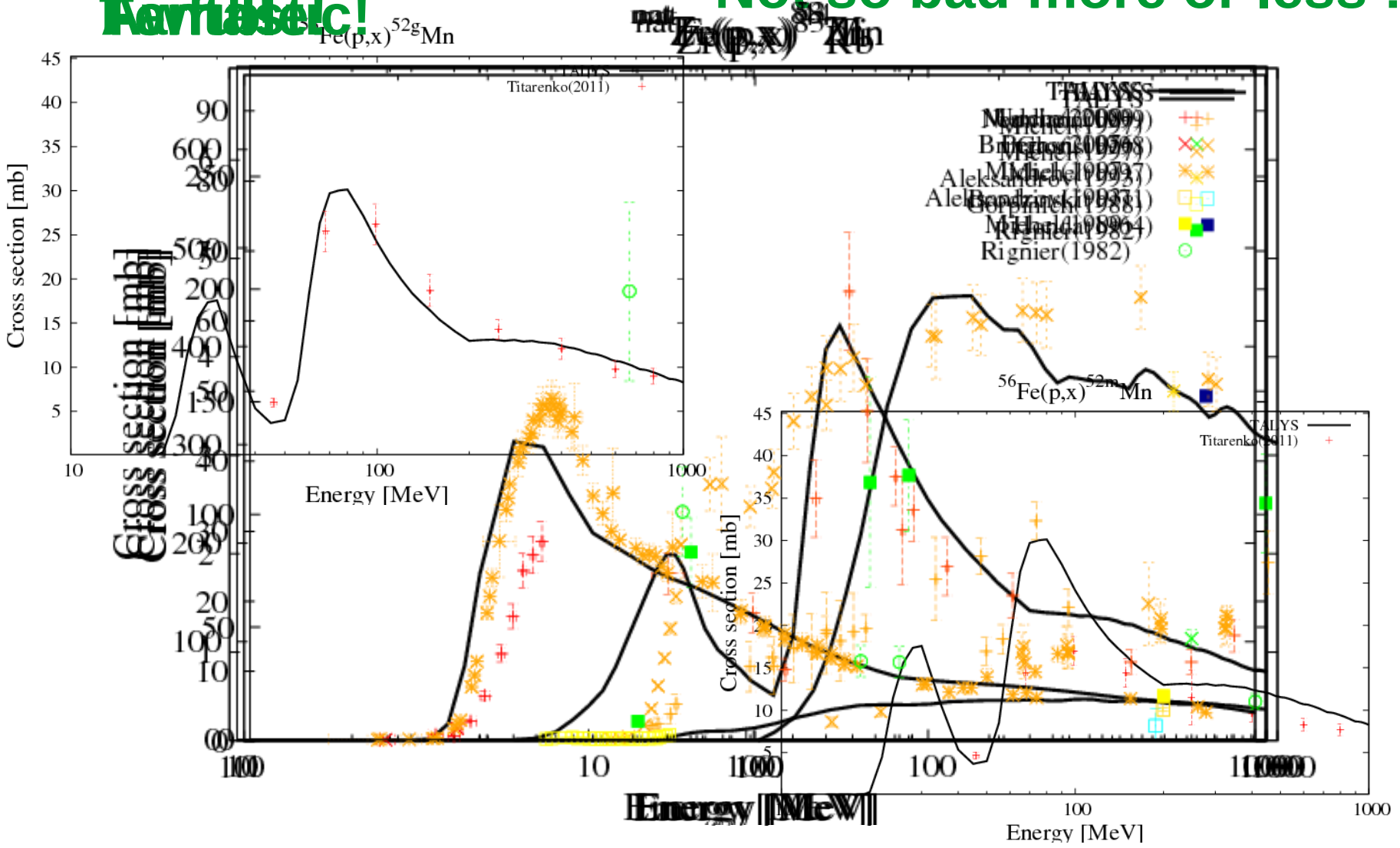
Coupling with GEF code

FEW EXAMPLES OF RESULTS

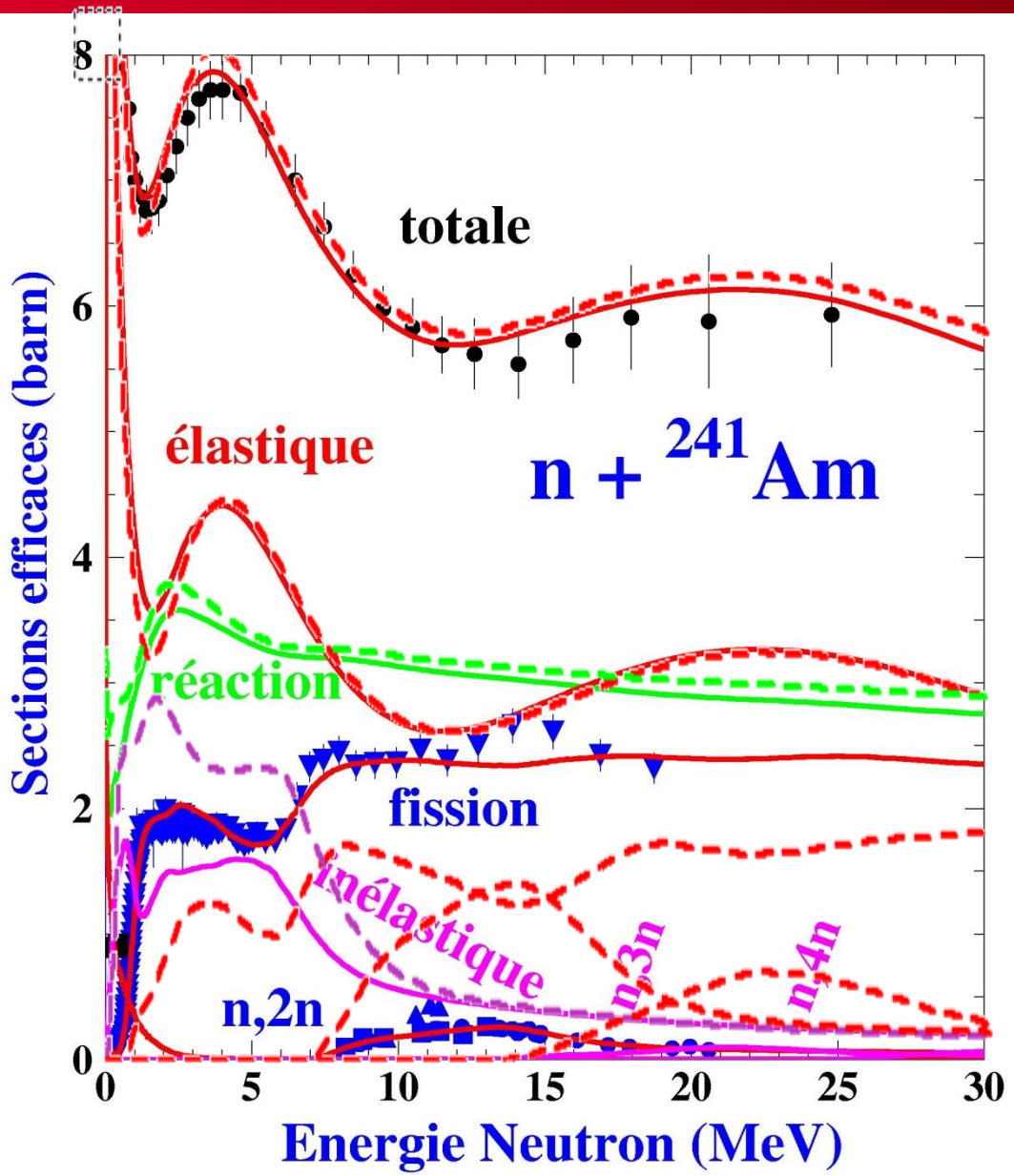
OBTAINED WITH TALYS

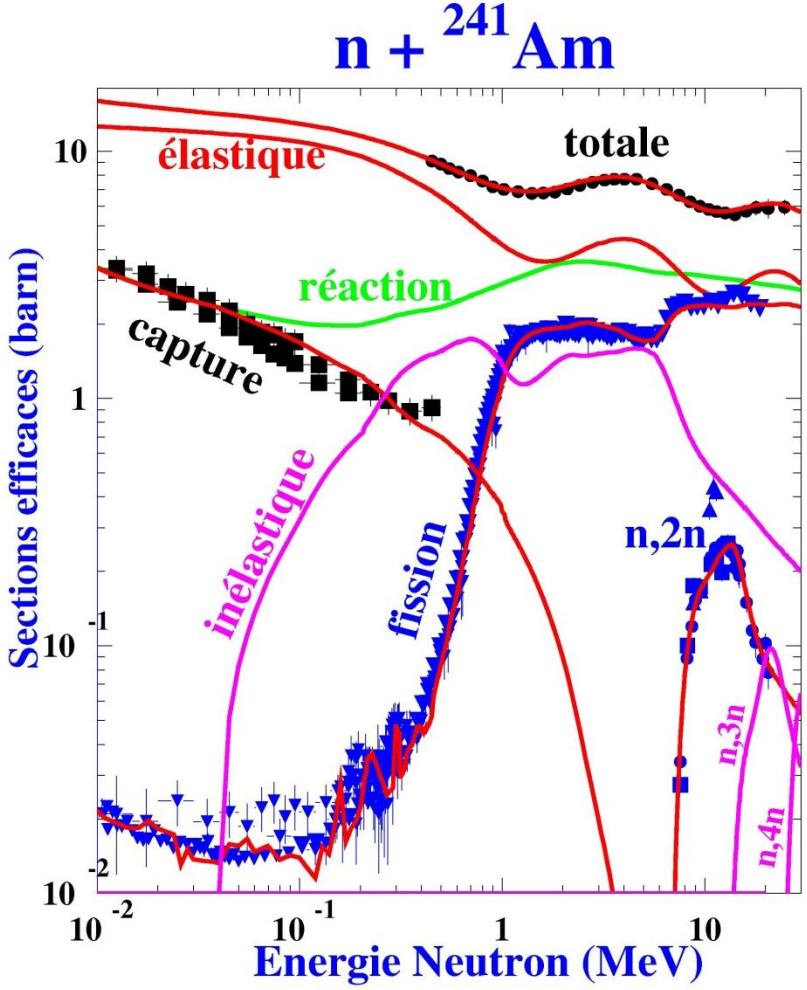
And finally: rather good!

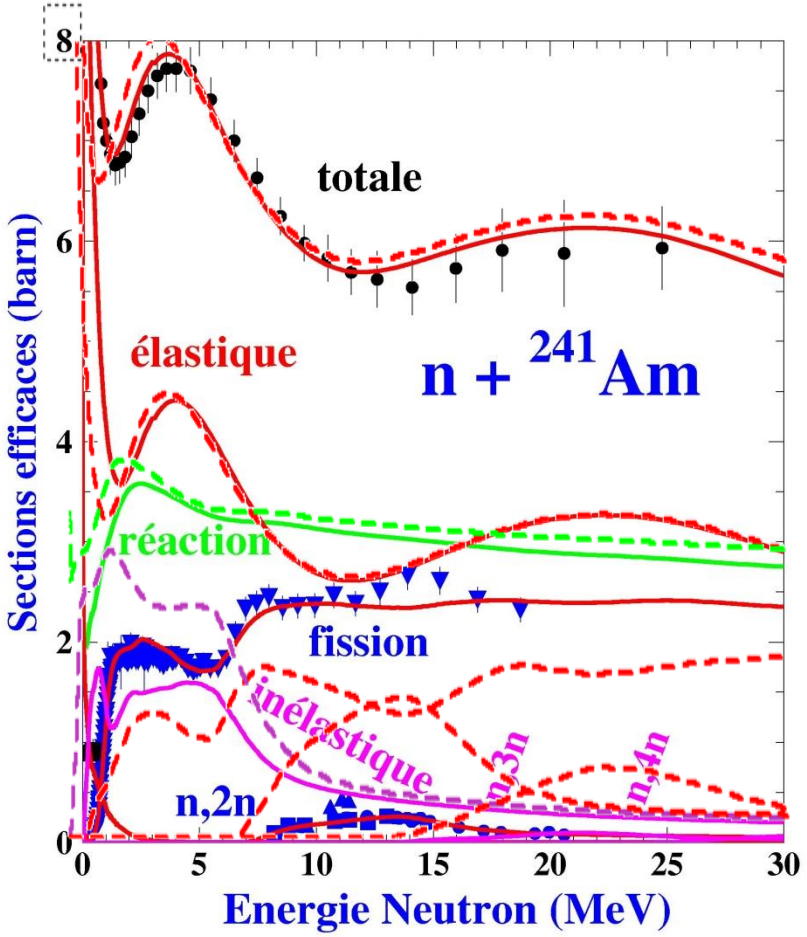
Not so bad more or less !



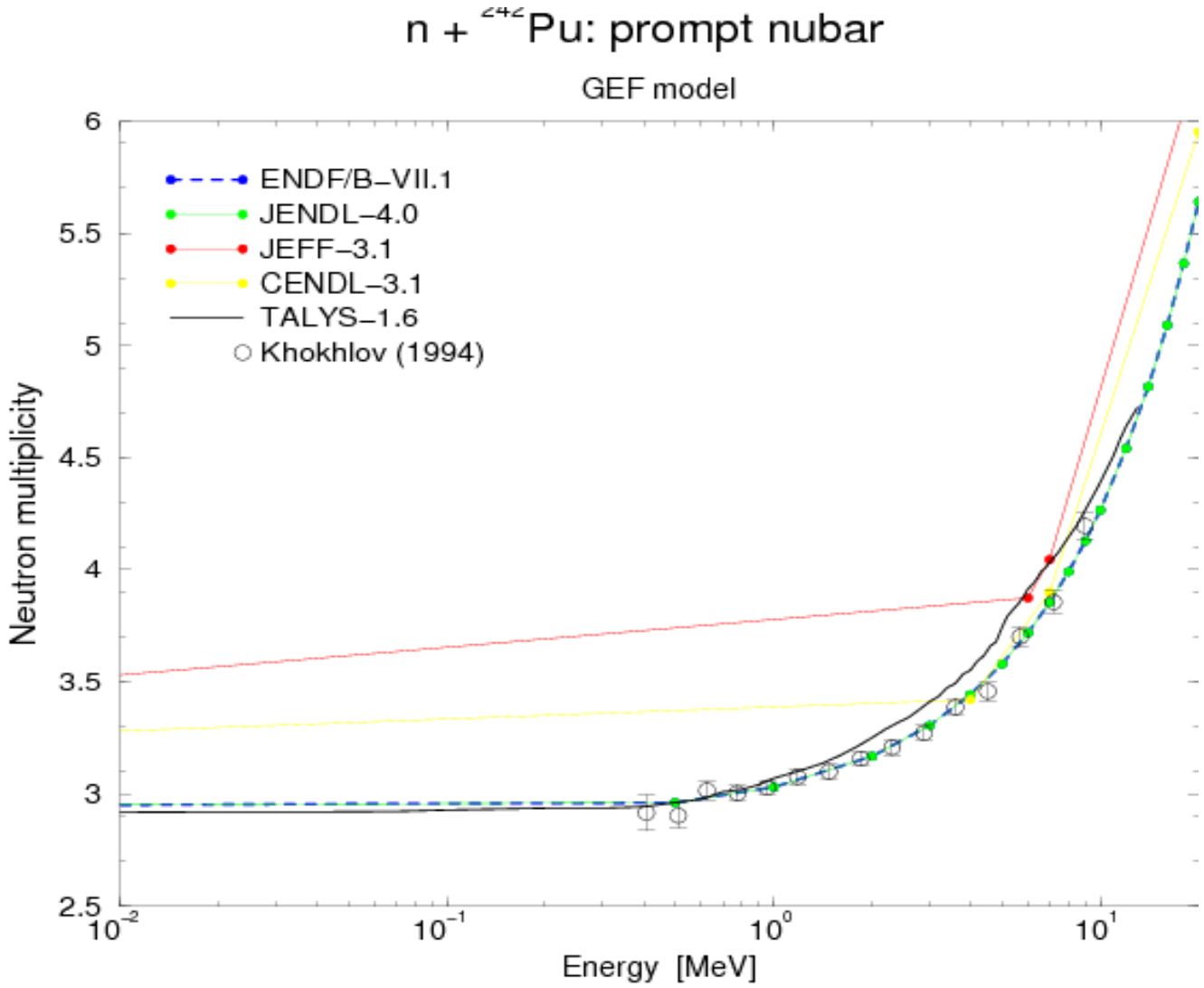
FISSION


totale
élastique
n + 241Am
réaction
fission
inélastique
n,3n
n,4n
n,2n
Sections efficaces (barn)
Energie Neutron (MeV)
0
2
4
6
8
0
5
10
15
20
25
30

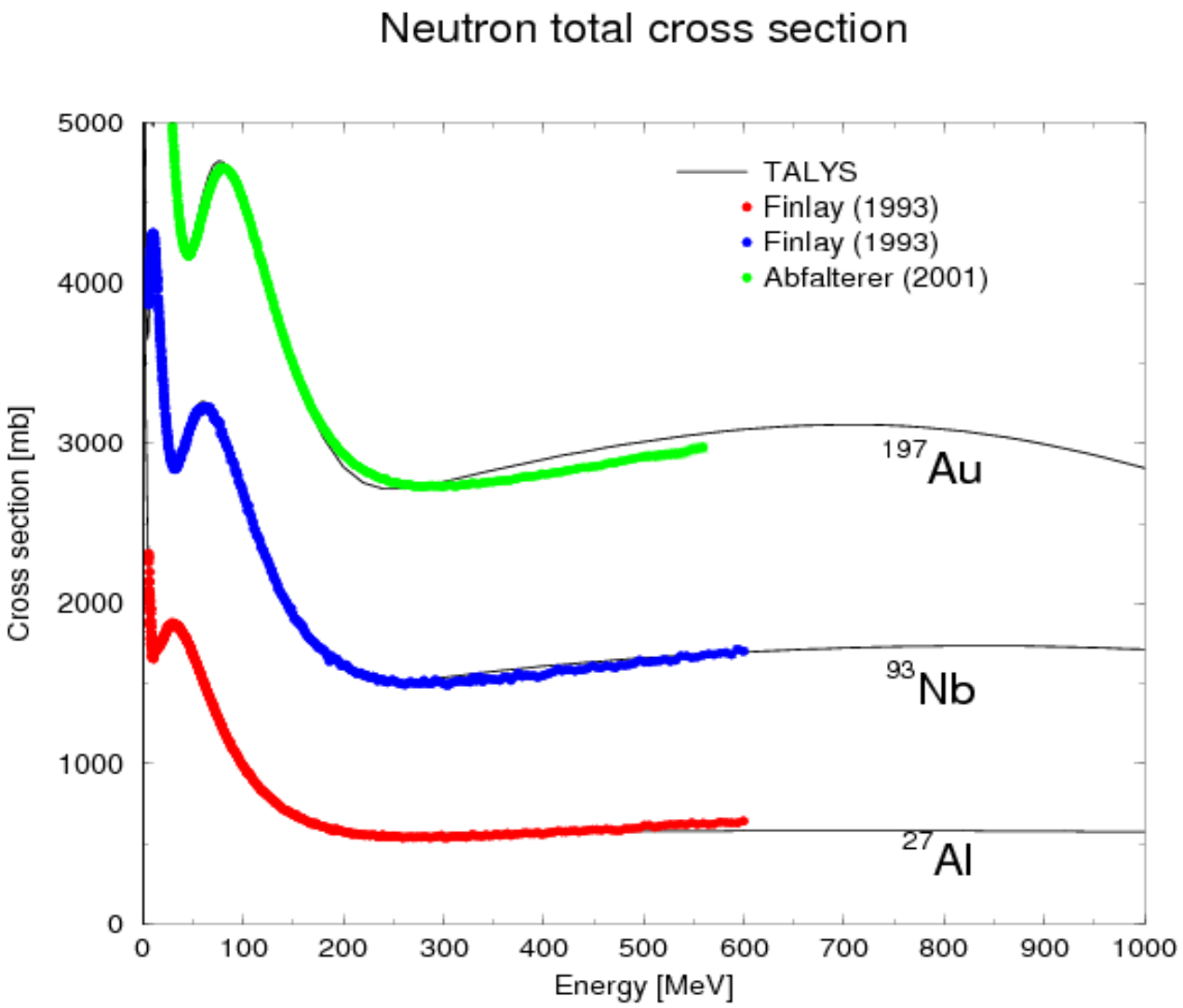

n + 241Am
élastique
totale
réaction
capture
inélastique
fission
n,2n
n,3n
n,4n
Sections efficaces (barn)
Energie Neutron (MeV)


totale
élastique
n + 241Am
réaction
fission
inélastique
n,2n
n,3n
n,4n
Sections efficaces (barn)
Energie Neutron (MeV)

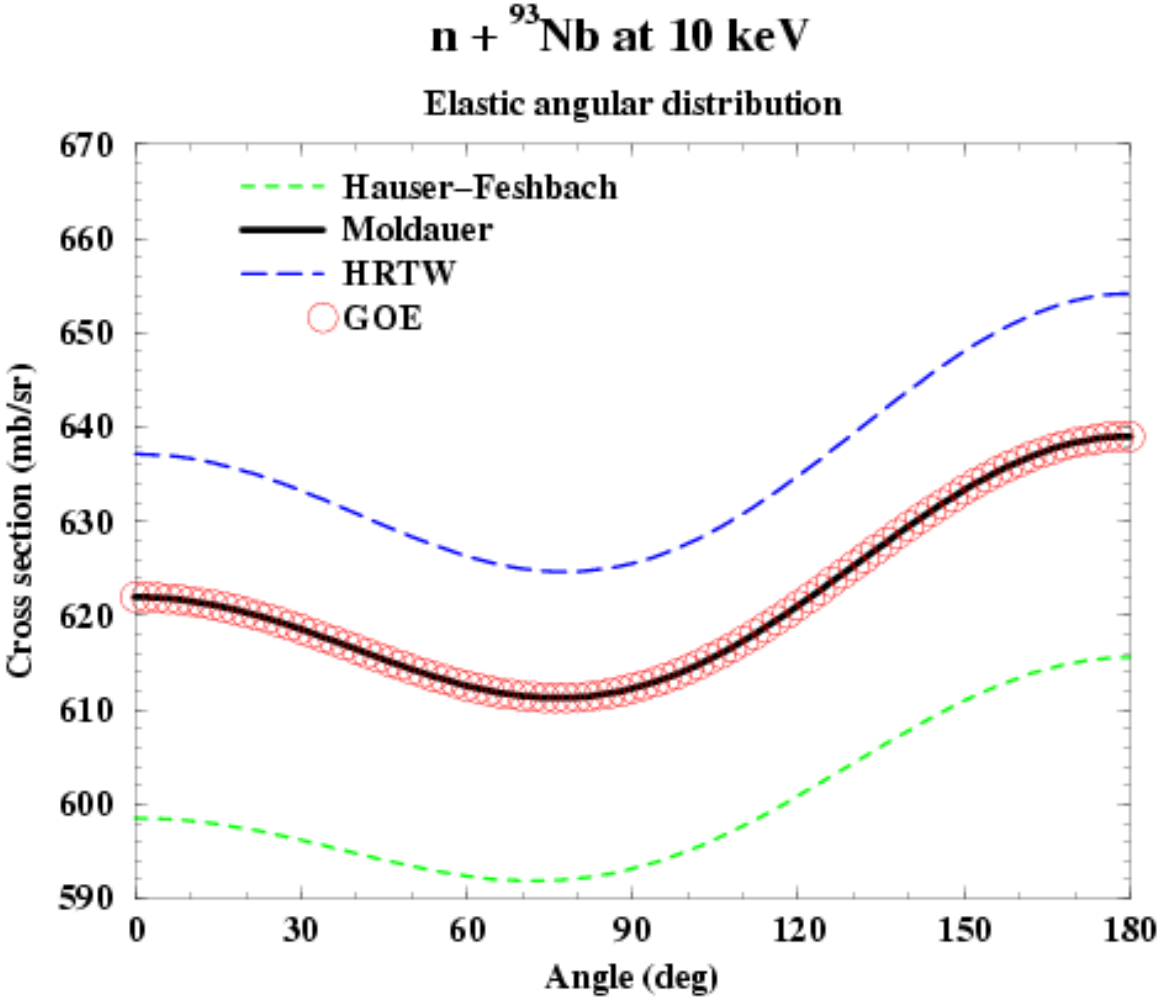
COUPLING WITH GEF



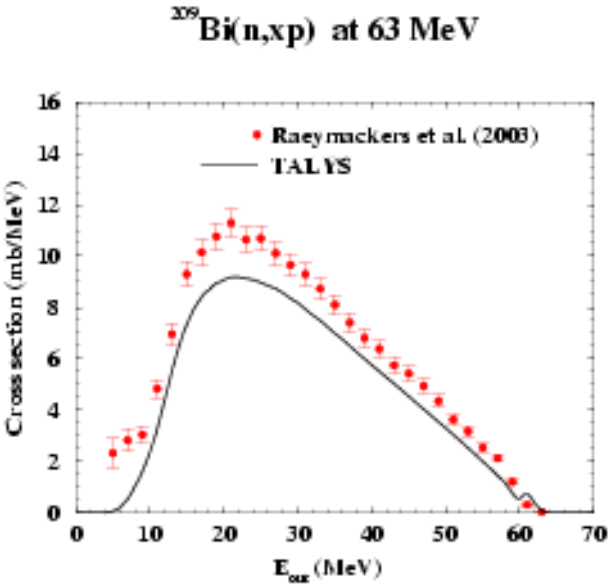
HIGH ENERGY

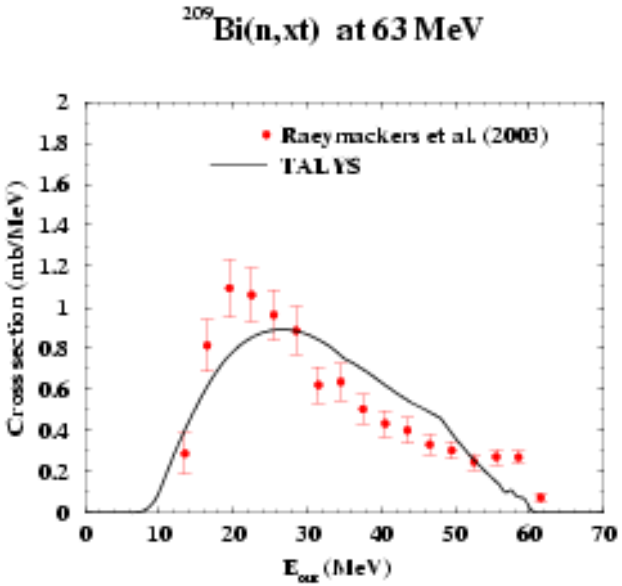

Neutron total cross section
TALYS
Finlay (1993)
Finlay (1993)
Abfalterer (2001)
197Au
93Nb
27Al
Cross section [mb]
Energy [MeV]
0
1000
2000
3000
4000
5000
0
100
200
300
400
500
600
700
800
900
1000

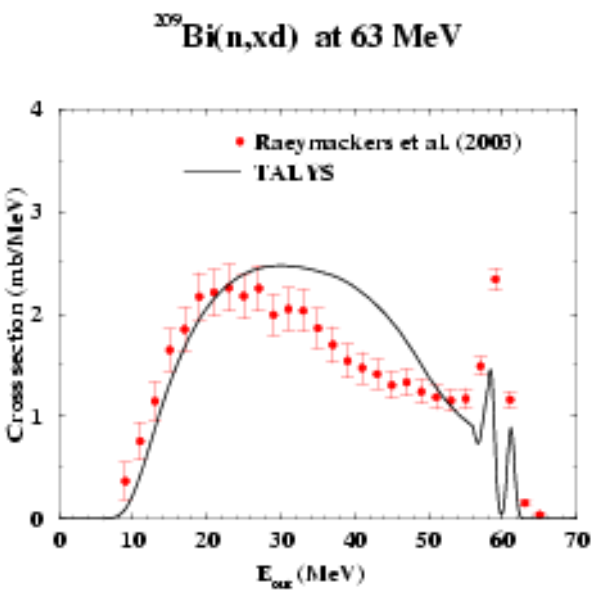
WIDTH FLUCTUATION COMPARISONS

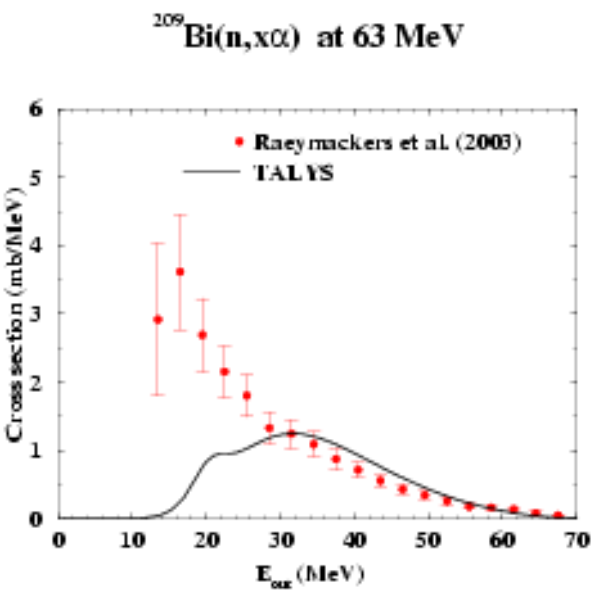


CONTINUUM SPECTRA

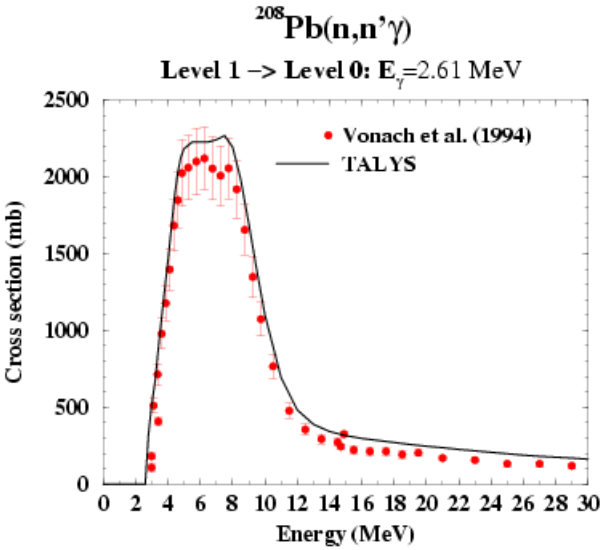


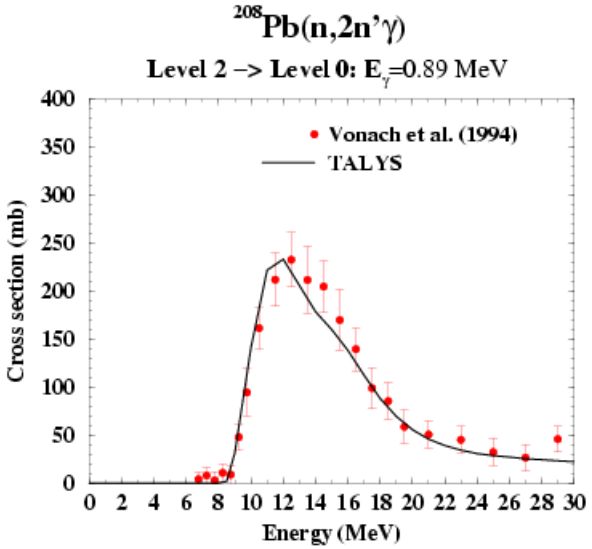


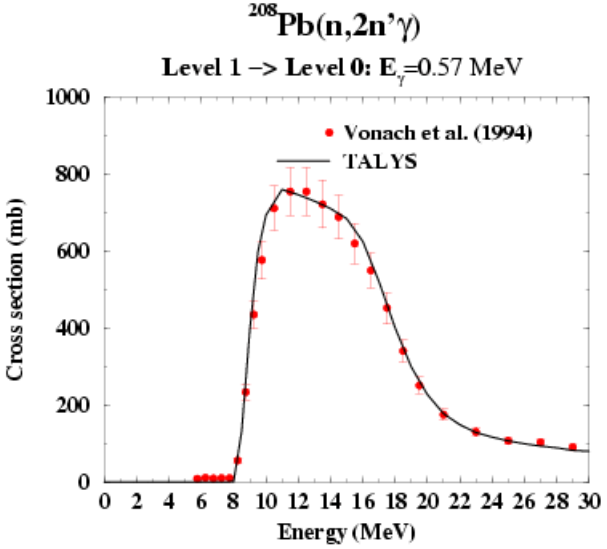




(n,xnγ) wich works !







Improvements still required !

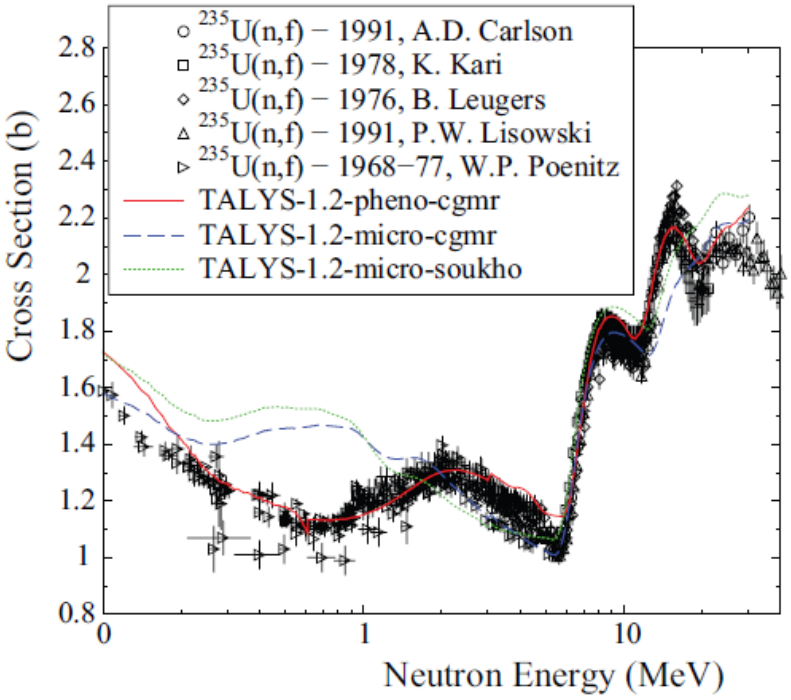


FIG. 11. (Color online) Total ^{235}U(n, f) cross section computed by TALYS-1.2 and compared to evaluated database values.

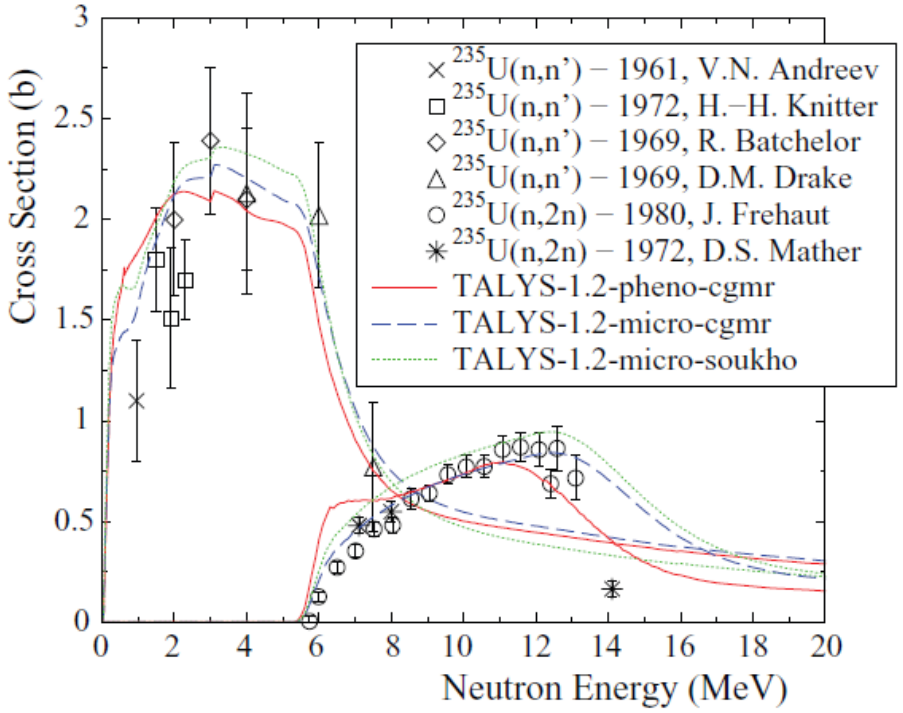


FIG. 12. (Color online) Total ^{235}U(n, n') and total ^{235}U(n, $2n$) cross section computed by TALYS-1.2 and compared to evaluated database values.

≈ OK for global cross sections

Improvements still required !

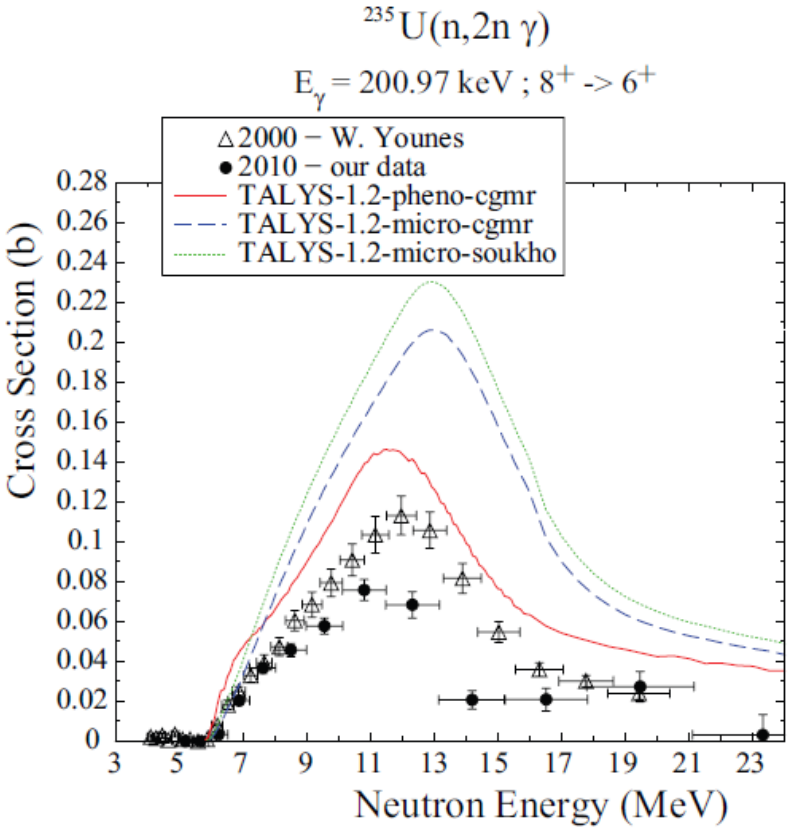


FIG. 9. (Color online) Total γ production cross section of the 200.97 keV transition from states $8^+ \rightarrow 6^+$ due to a $^{235}U(n, 2n)^{234}U^*$ reaction compared to TALYS-1.2 predictions and prior measurements. For this work, reported uncertainties are the combination of the statistical and systematic errors (see Sec. III F).

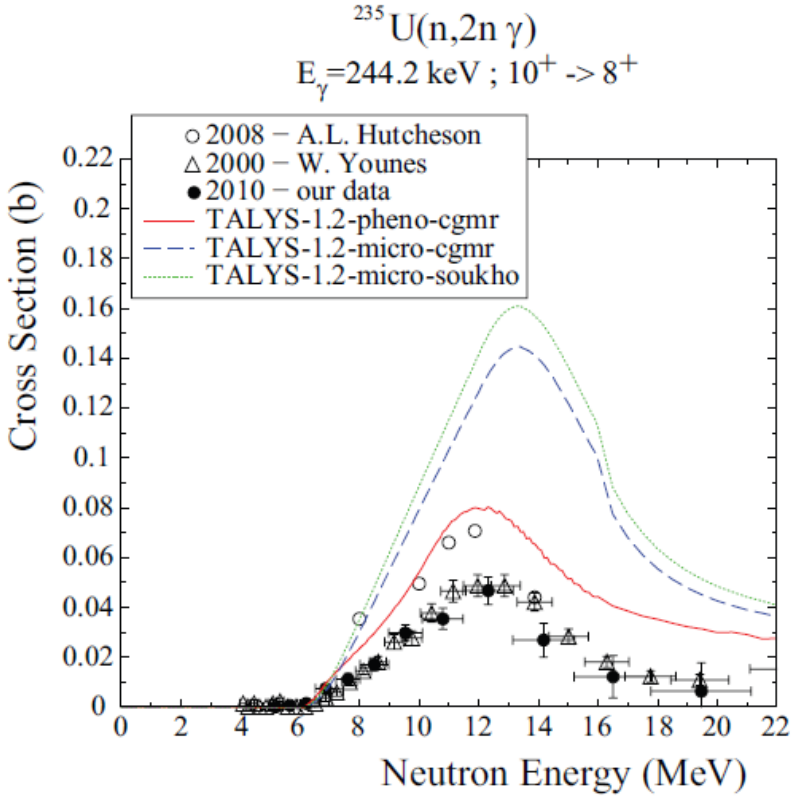


FIG. 10. (Color online) Total γ production cross section of the 244.2 keV transition from states $10^+ \rightarrow 8^+$ due to a $^{235}U(n, 2n)^{234}U^*$ reaction compared to TALYS-1.2 predictions and other experimental measurements. For this work, reported uncertainties are the combination of the statistical and systematic errors (see Sec. III F).

Still work to do for subtle cross sections

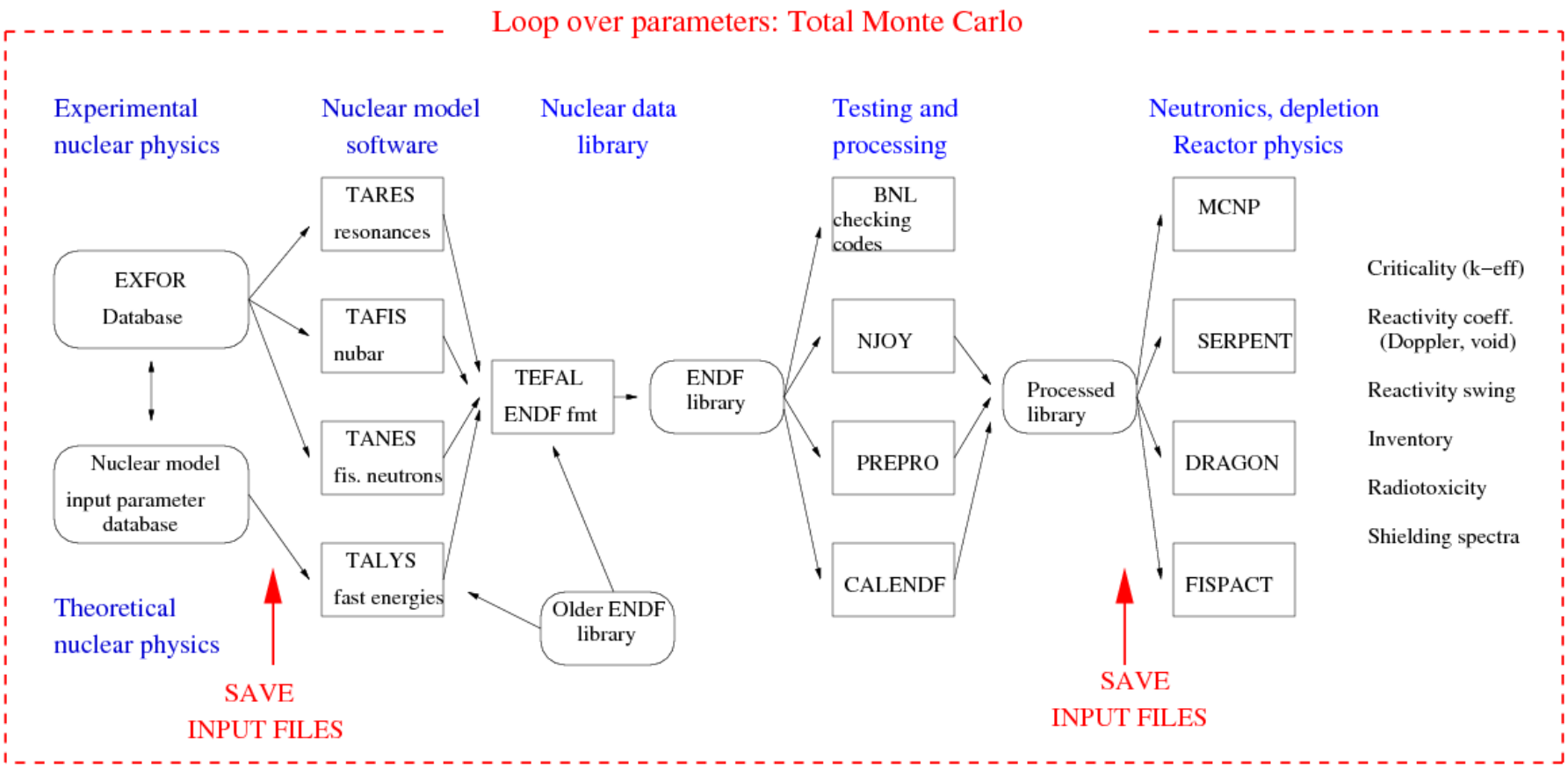
WHAT REMAINS TO BE DONE ?

PERSPECTIVES

- Coupling with microscopic models
  - . Deformed JLM (almost ok)
  - . Densités p-h
  - . Pré-équilibre microscopique

- Total Monte Carlo : Done !

Automating nuclear reactions: Total Monte Carlo



PERSPECTIVES

- Coupling with microscopic models
  - . Deformed JLM (almost ok)
  - . Densités p-h
  - . Pré-équilibre microscopique

- Total Monte Carlo : Done !

- A.J.K : “ Now that I have done it all, I know how I Should have done it, so let’s do it ! ”

TOWARDS TALYS 2.0

- Full rewrite in Fortran-90/95/03/08:
  - Work has already started: input and create_nucleus(Z,A)
- Integration of TASMAN:
  - statistics
  - optimization (parameter search)
  - sensitivities
  - uncertainties
  - covariances
  - Total Monte Carlo
- Integration of TEFAL:
  - Complete ENDF-6 formatting from MF1 to MF40