DE LA RECHERCHE À L'INDUSTRIE

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# Nuclear reaction modeling using the TALYS code: energy applications

TRIESTE 2014 – S. Hilaire & The TALYS Team – 24/09/2014

# Content

## - Introduction

## - General features about nuclear reactions

- Time scales and associated models
- Types of data needed
- Data format = f (users)

## - Nuclear Models

- Basic structure properties
- Optical model
- Pre-equilibrium model
- Compound Nucleus model
- Miscellaneous : level densities, fission, capture

## - From in depth analysis to large scale production with TALYS

- General features about TALYS
- Fine tuning and accuracy
- Global systematic approaches

## - What remains to be done ?

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YESTERDAY

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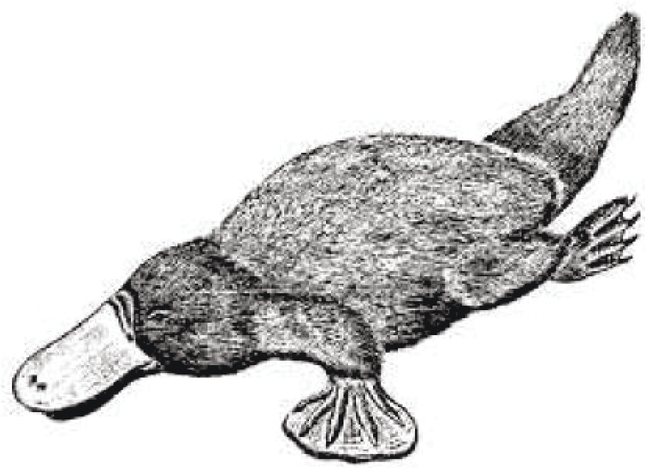
TODAY

# The bible today

# TALYS-1.6

New Edition December 23, 2013

*A nuclear reaction program*



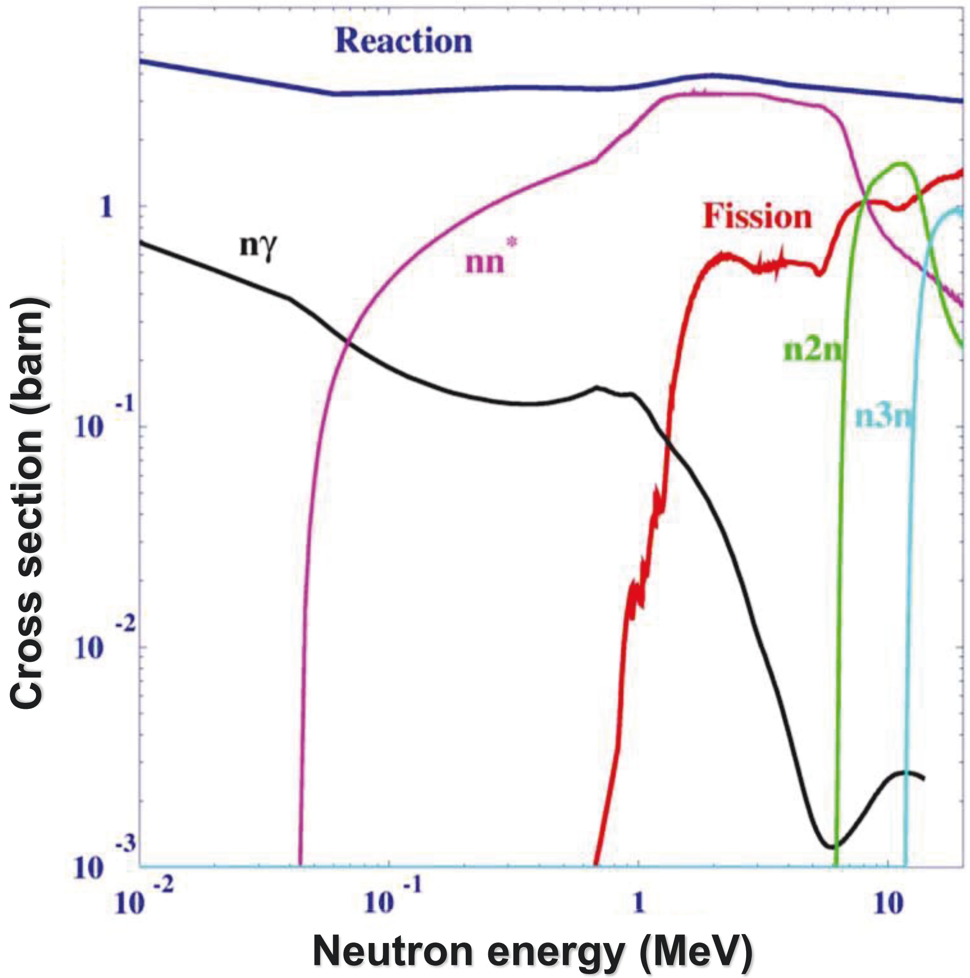
PLATYPUS

*User Manual*

**Arjan Koning**
**Stephane Hilaire**
**Stephane Goriely**

# REACTION MODELS & REACTION CHANNELS (REMINDER)

$n + {}^{238}U$




**Optical model**

**+**

**Statistical model**

**+**

**Pre-equilibrium model**

$$\sigma_R = \sigma_d + \sigma_{PE} + \sigma_{CN}$$

$$= \sigma_{nn'} + \sigma_{nf} + \sigma_{n\gamma} + \ldots$$

# FROM IN DEPTH ANALYSIS TO LARGE SCALE PRODUCTION WITH TALYS

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# GENERAL FEATURES
## 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**

# GENERAL FEATURES
# 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
# 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

# GENERAL FEATURES
# 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 ??

. 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)

# GENERAL FEATURES
## 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

# GENERAL FEATURES
# 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.**

# GENERAL FEATURES
# TALYS versions online

## http://www.talys.eu

**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, $\gamma$ 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

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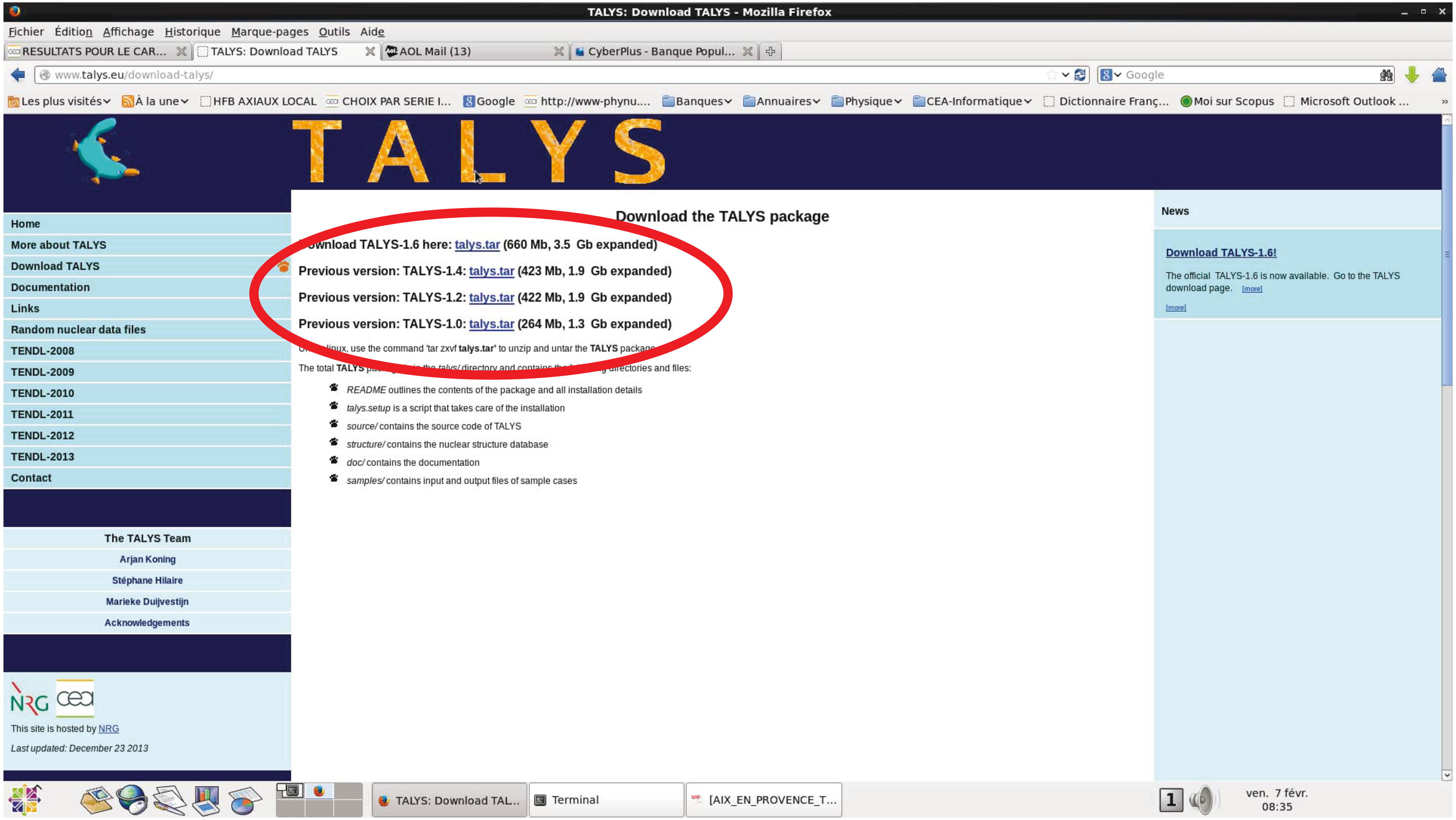
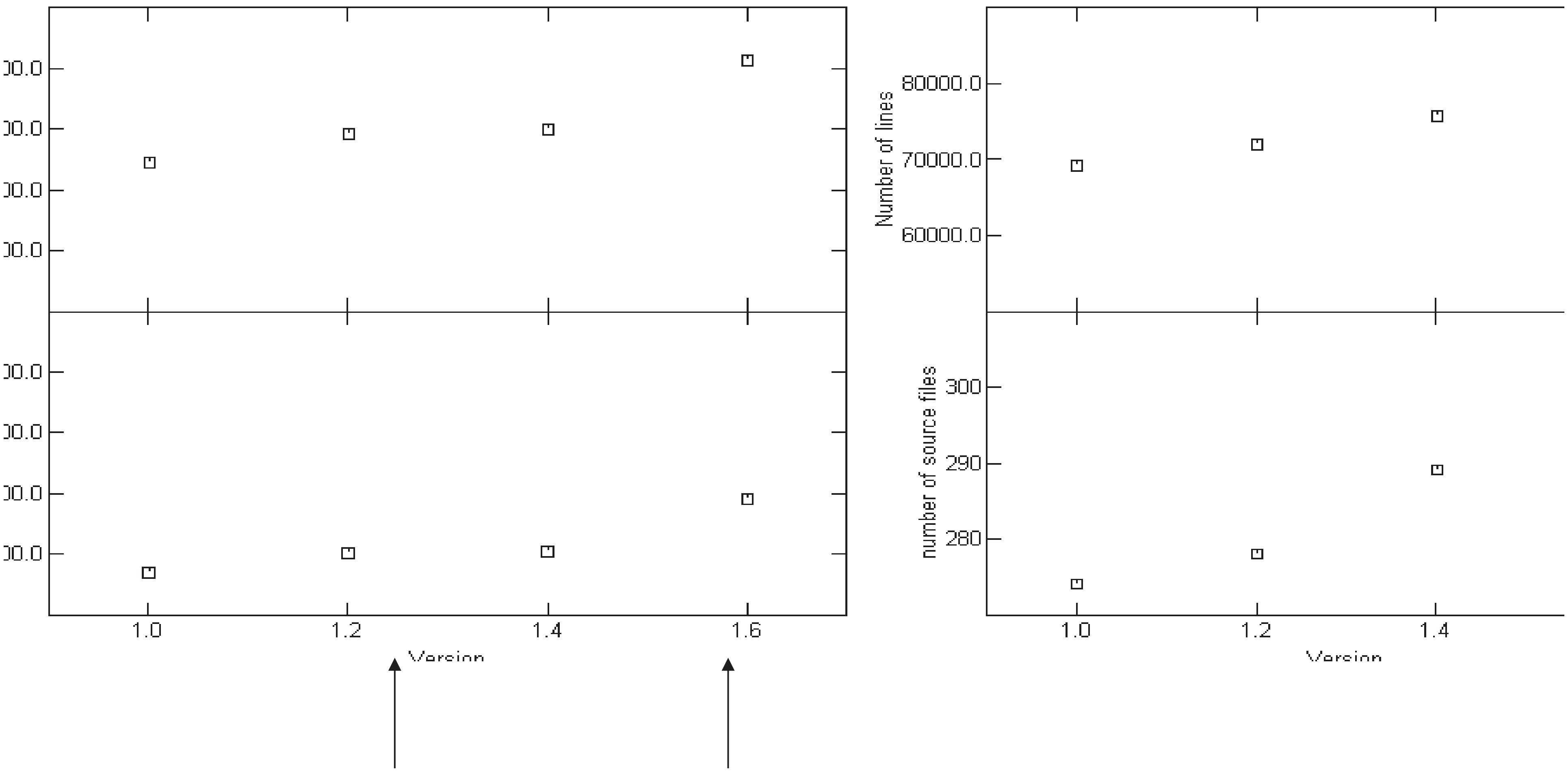
# TALYS versions online

## http://www.talys.eu



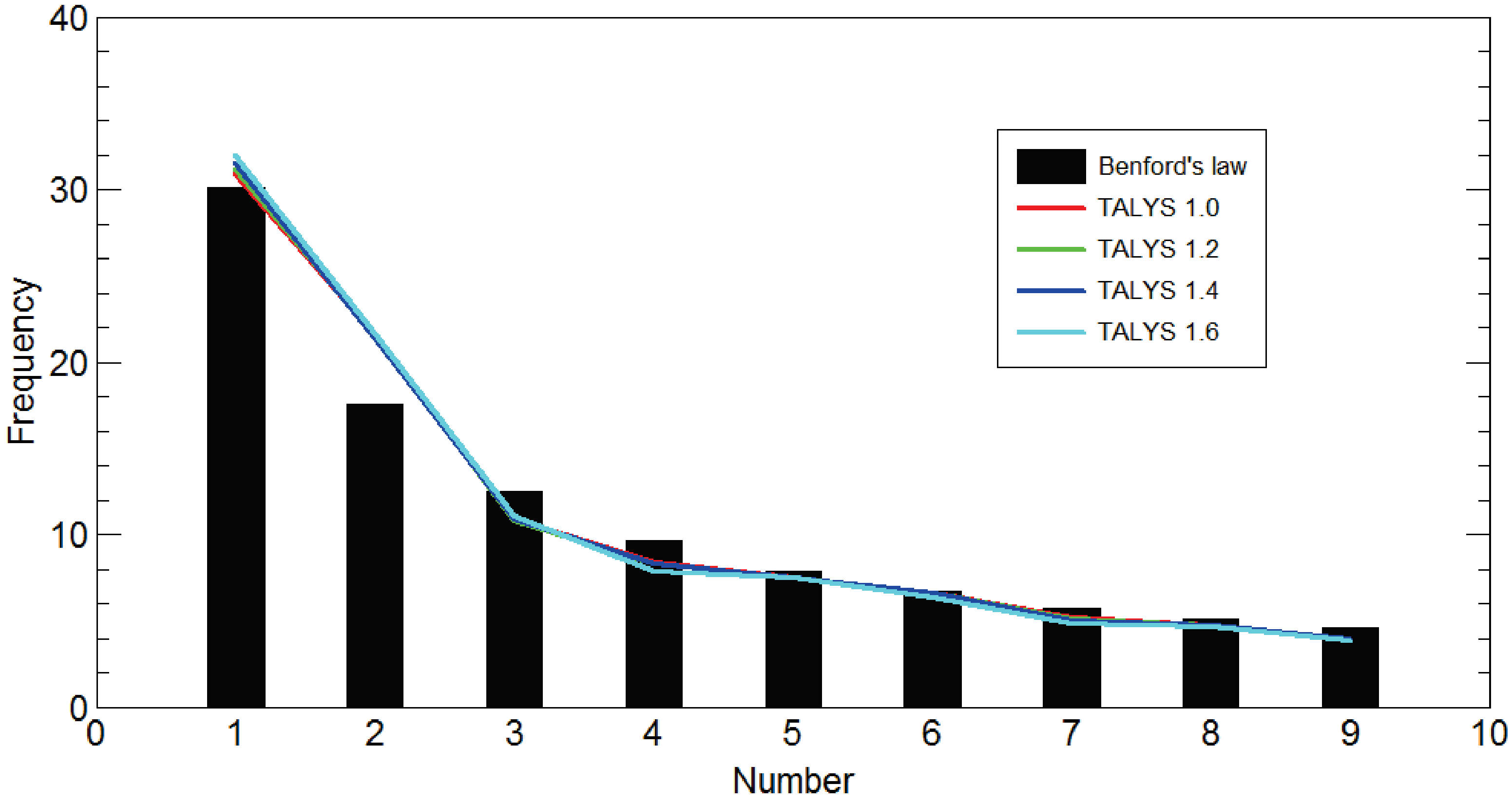
# GENERAL FEATURES
# TALYS statistics (1/2)




Inclusion of ph lds

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

# GENERAL FEATURES
# TALYS statistics (2/2)

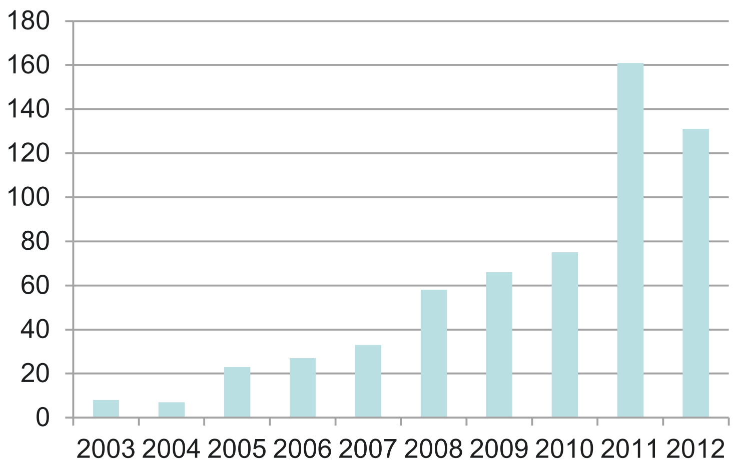


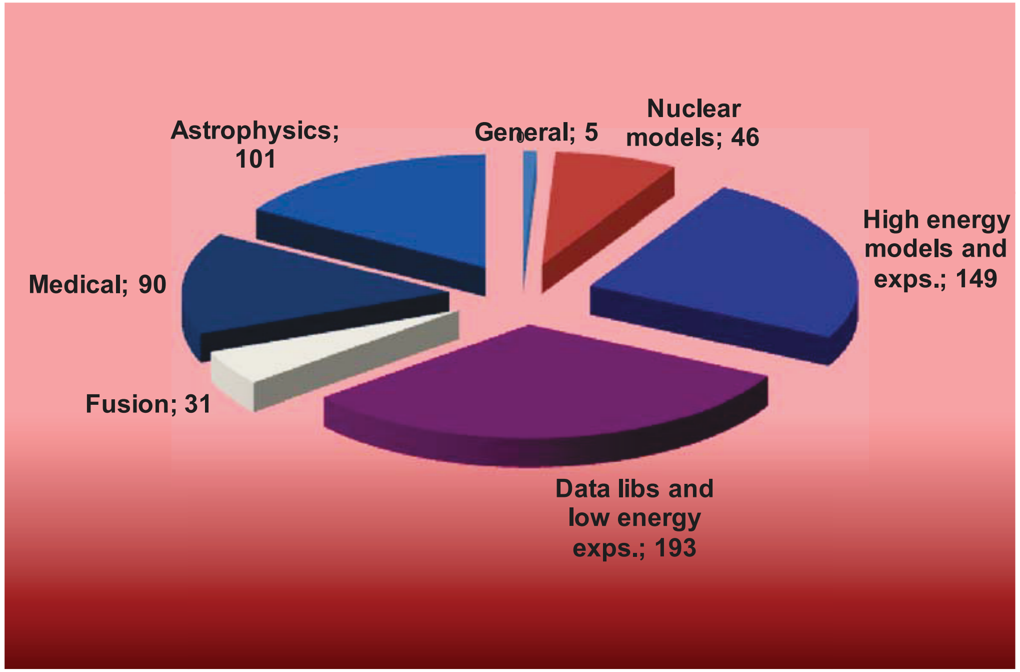

**TALYS obeys the Benford's law : no intentional scientific fraud**

# GENERAL FEATURES
# TALYS users and publications

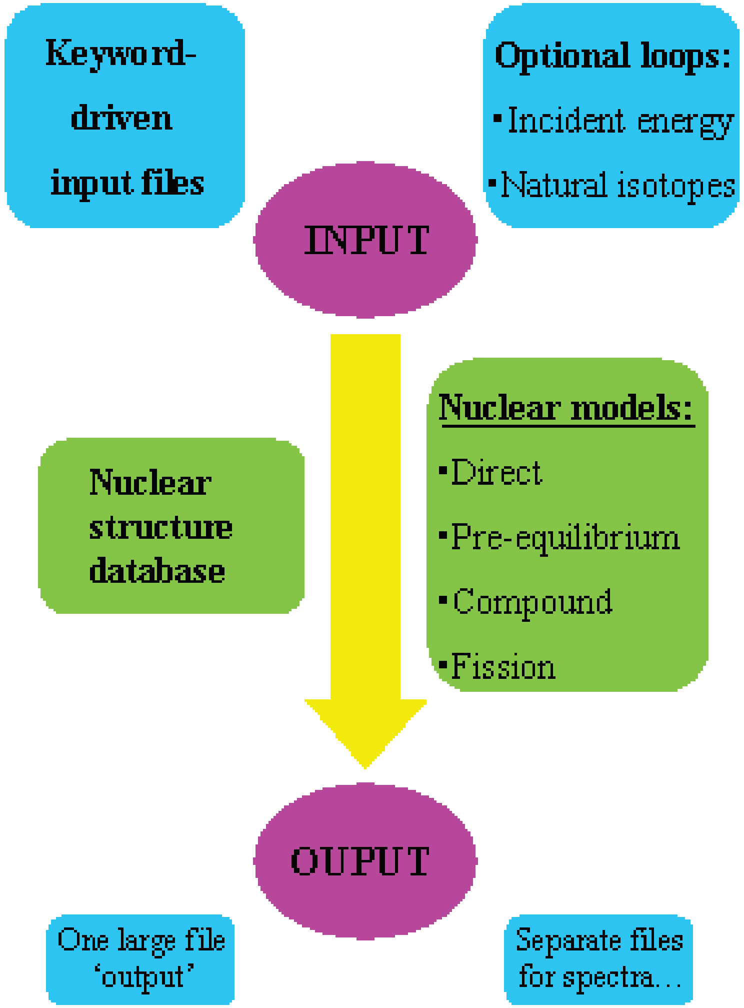
- User feedback via talys mailing list : info@talys.eu to be added to mailing list
: talys-l@nrg.eu to inform mailing list

## PUBLICATIONS



# GENERAL FEATURES
# TALYS Scheme



# GENERAL FEATURES
# 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 $\gamma$-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

## - 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 $(n,\gamma)$, (n,2n), (n,p), (n,d) and $(n,\alpha)$ 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)

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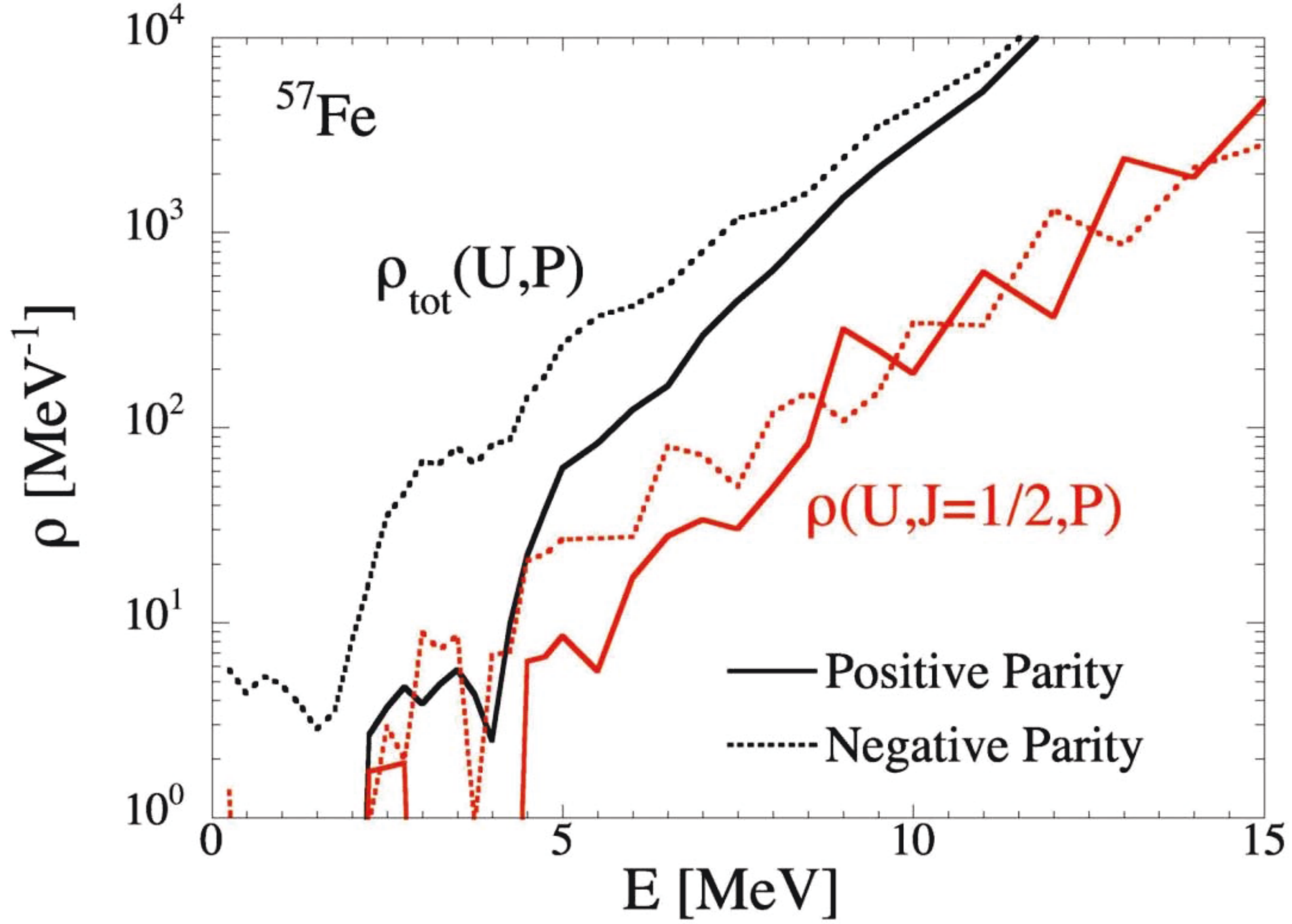
# FINE TUNING AND ACCURACY

- Non statistical effects in nuclear level densities
- Decay spin selection rules at work
- Coherent modeling of fission cross sections
- Predictions for unstable target
- Microscopic modeling of fission cross sections
- Coherent microscopic modeling of fission cross sections
- Microscopic pre-equilibrium modeling of cross sections

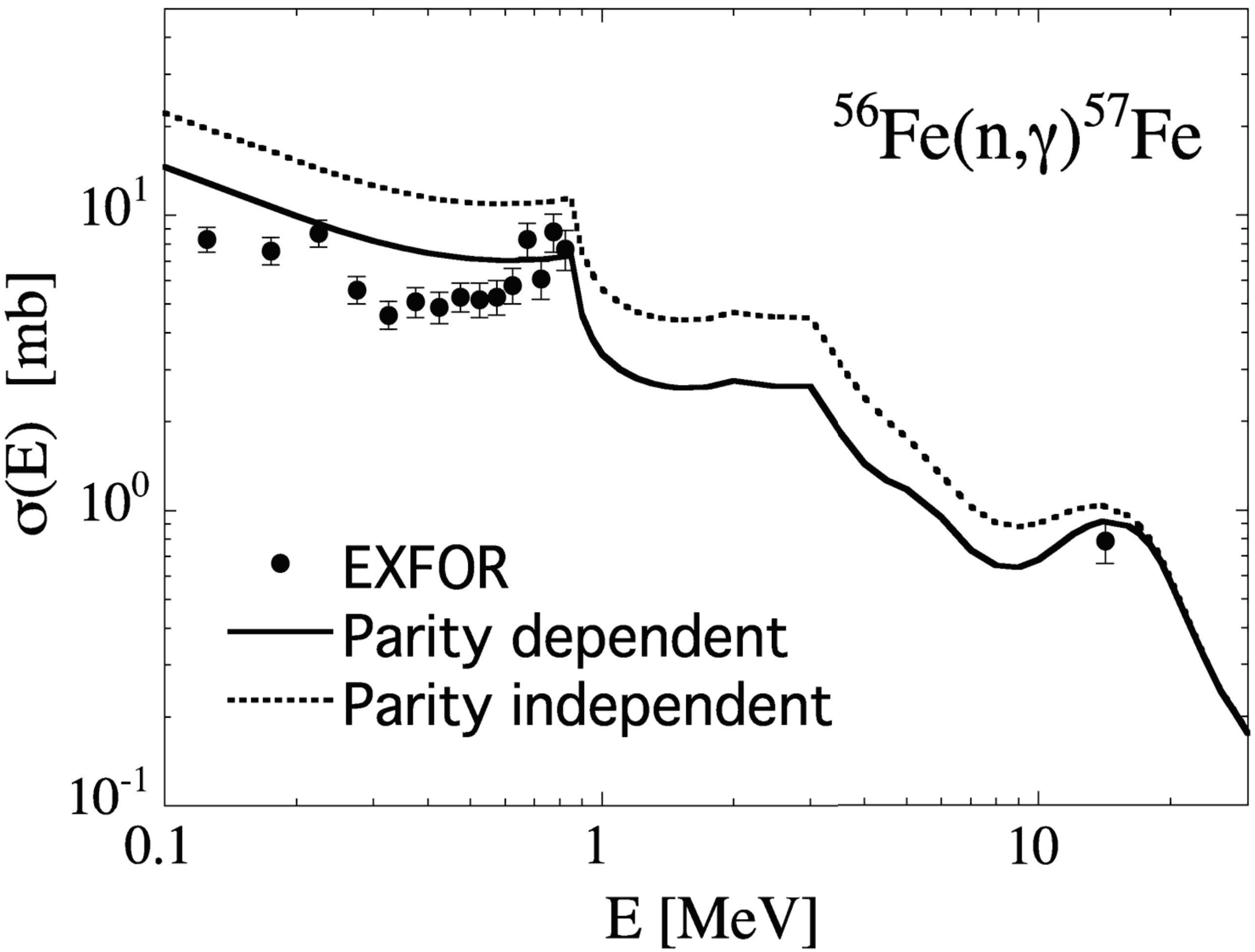
# FINE TUNING AND ACCURACY
# Non statistical effects in nuclear level densities (1/4)

***Talys deals with realistic (non statistical) spin & parity distributions***



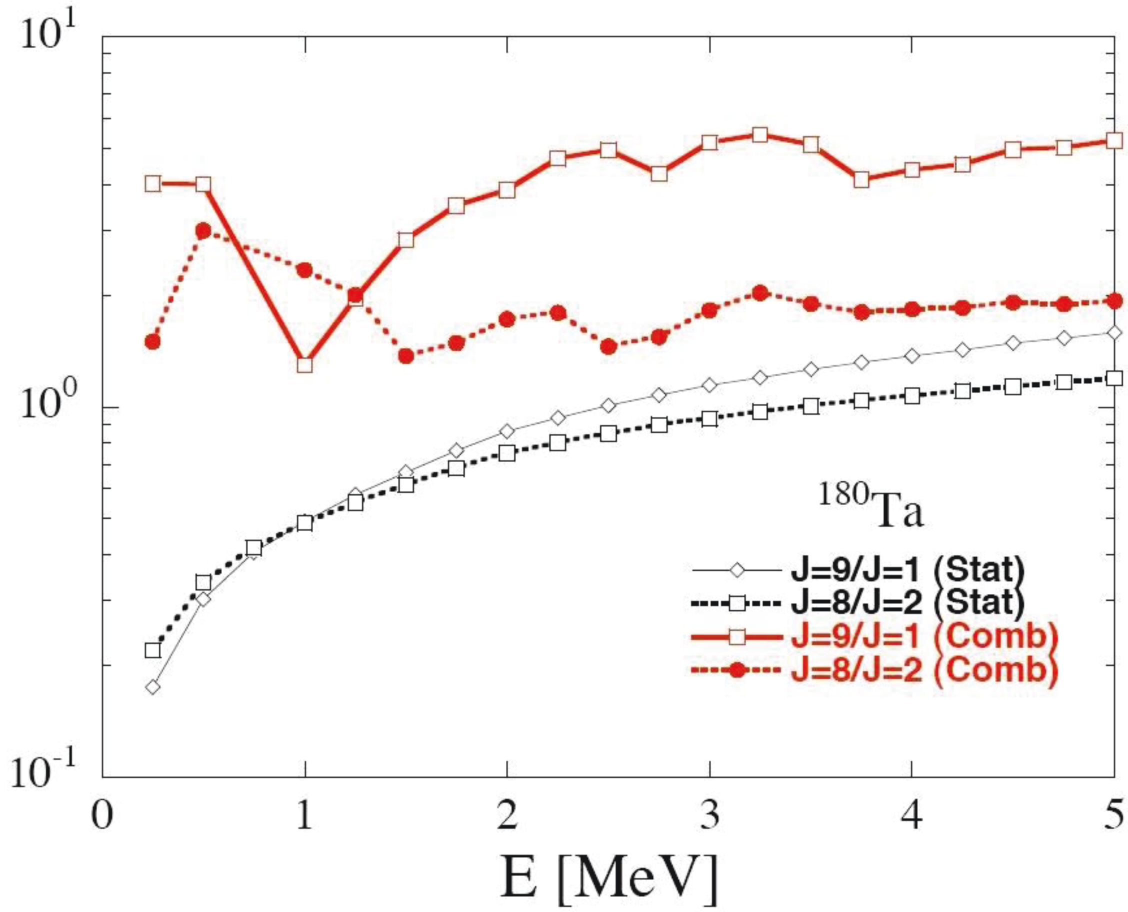
# FINE TUNING AND ACCURACY
## Non statistical effects in nuclear level densities (2/4)

***Talys deals with realistic (non statistical) spin & parity distributions***



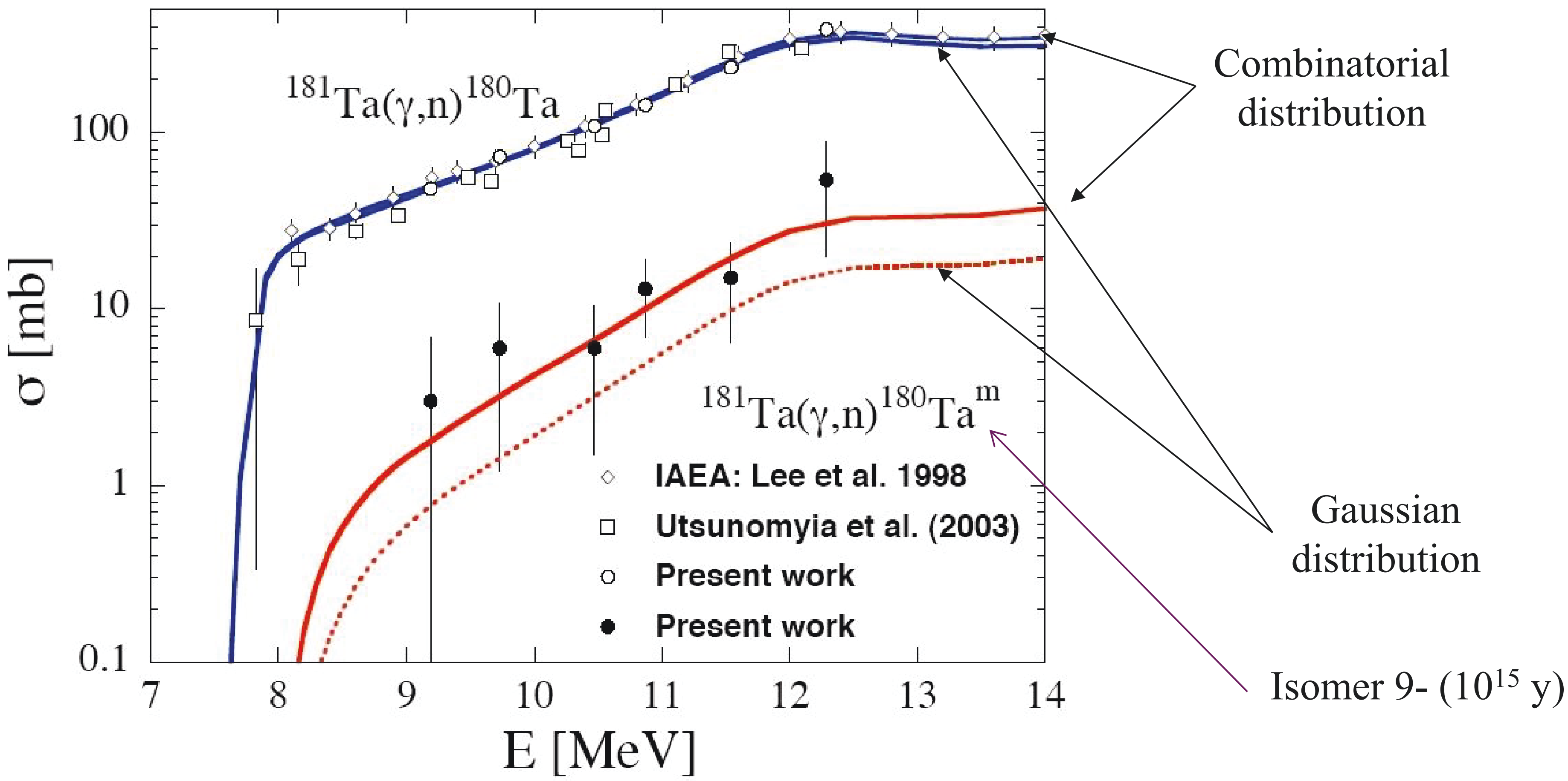
# FINE TUNING AND ACCURACY
## Non statistical effects in nuclear level densities (3/4)

**Talys deals with realistic (non statistical) spin & parity distributions**




➡ **Non-statistical feature imply significant deviations from the usual gaussian spin dependence**

## Talys deals with realistic (non statistical) spin & parity distributions

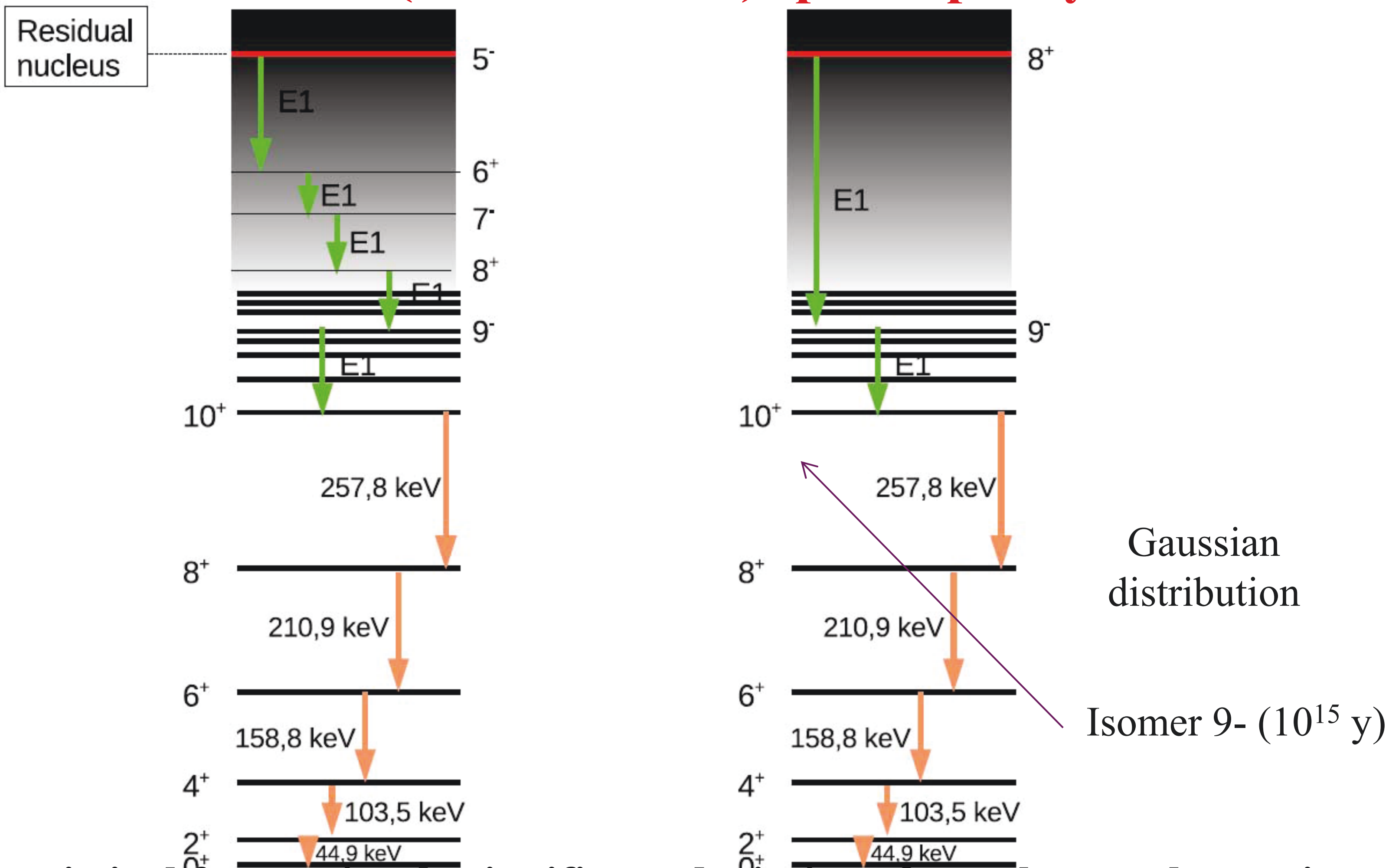



➡ **Non-statistical feature imply significant deviations from the usual gaussian spin dependence which have significant impact on isomeric production**

*See PRL 96 (2006) 192501 for details*

# FINE TUNING AND ACCURACY
## Non statistical effects in nuclear level densities (4/4)

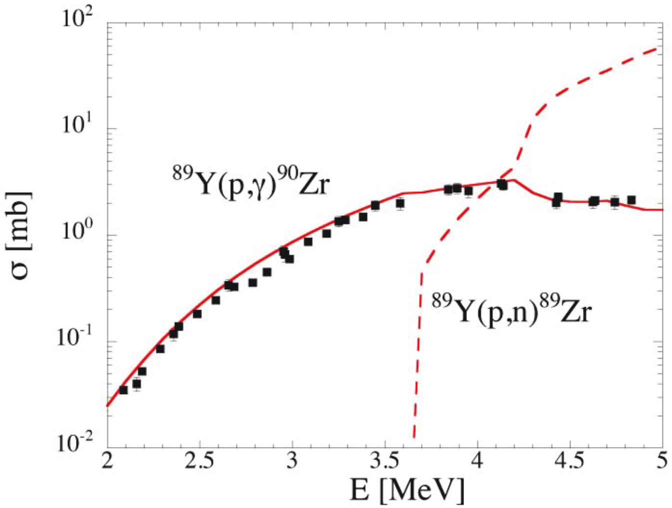
**Talys deals with realistic (non statistical) spin & parity distributions**




➡ **Non-statistical feature imply significant deviations from the usual gaussian spin dependence which have significant impact on isomeric production**

*See PRL 96 (2006) 192501 for details*

# FINE TUNING AND ACCURACY
# Decay spin selection rules at work (1/1)




$^{89}$Y Ground state : $1/2^+$

$^{89}$Y (p,n) $^{89}$Zr threshold = 3,65 MeV

Transmission coefficients incident proton at 4.5 MeV :

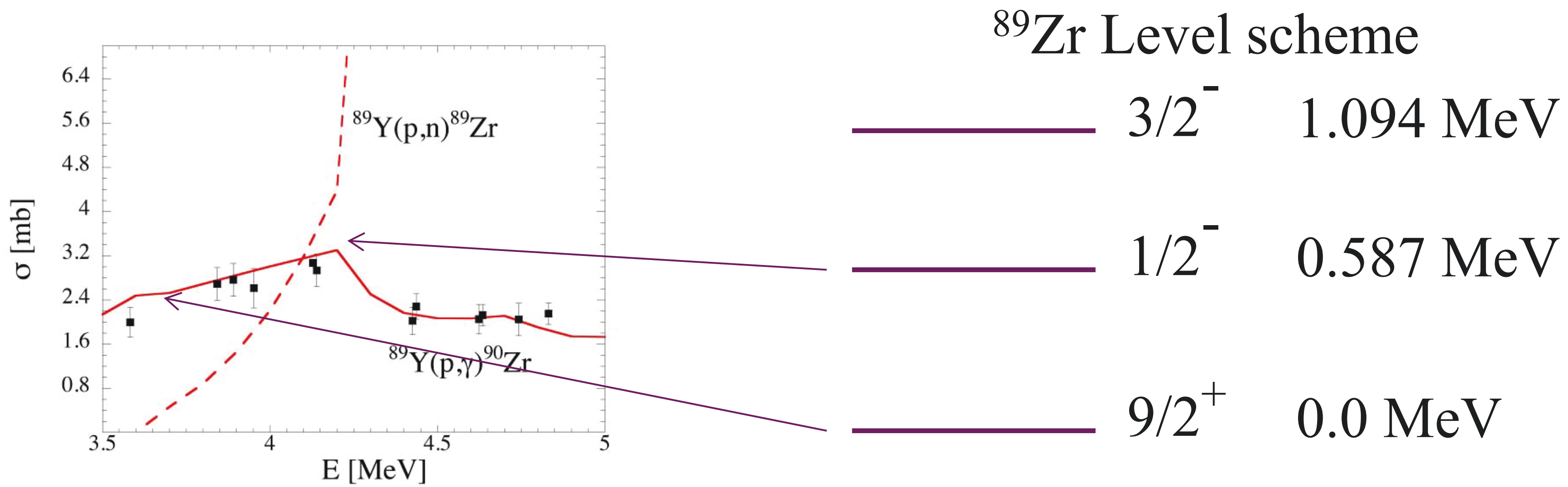
60 % l=0 ⇒ CN spin $0^+$, $1^+$

35 % l=1 ⇒ CN spin $0^-$, $1^-$, $2^-$

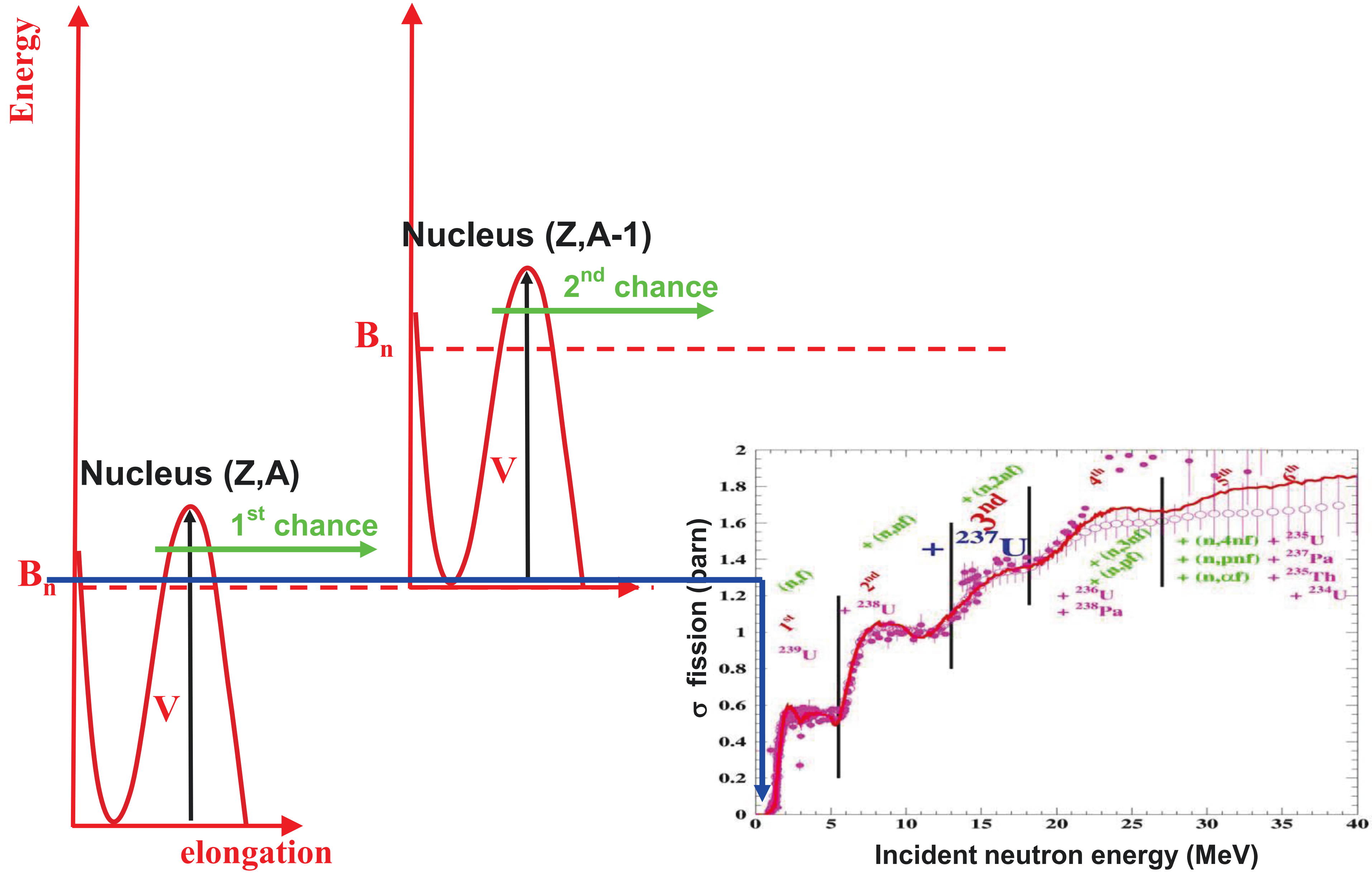
Transmission coefficients outgoing neutron at 1.0 MeV :

70 % l=1 ⇒ CN spin $1/2^-$, $3/2^-$, $5/2^-$, $1/2^+$, $3/2^+$, $5/2^+$, $7/2^+$

25 % l=0 ⇒ CN spin $1/2^-$, $3/2^-$, $5/2^-$, $1/2^+$, $3/2^+$



# FINE TUNING AND ACCURACY
## Coherent modeling of fission cross sections (1/3)



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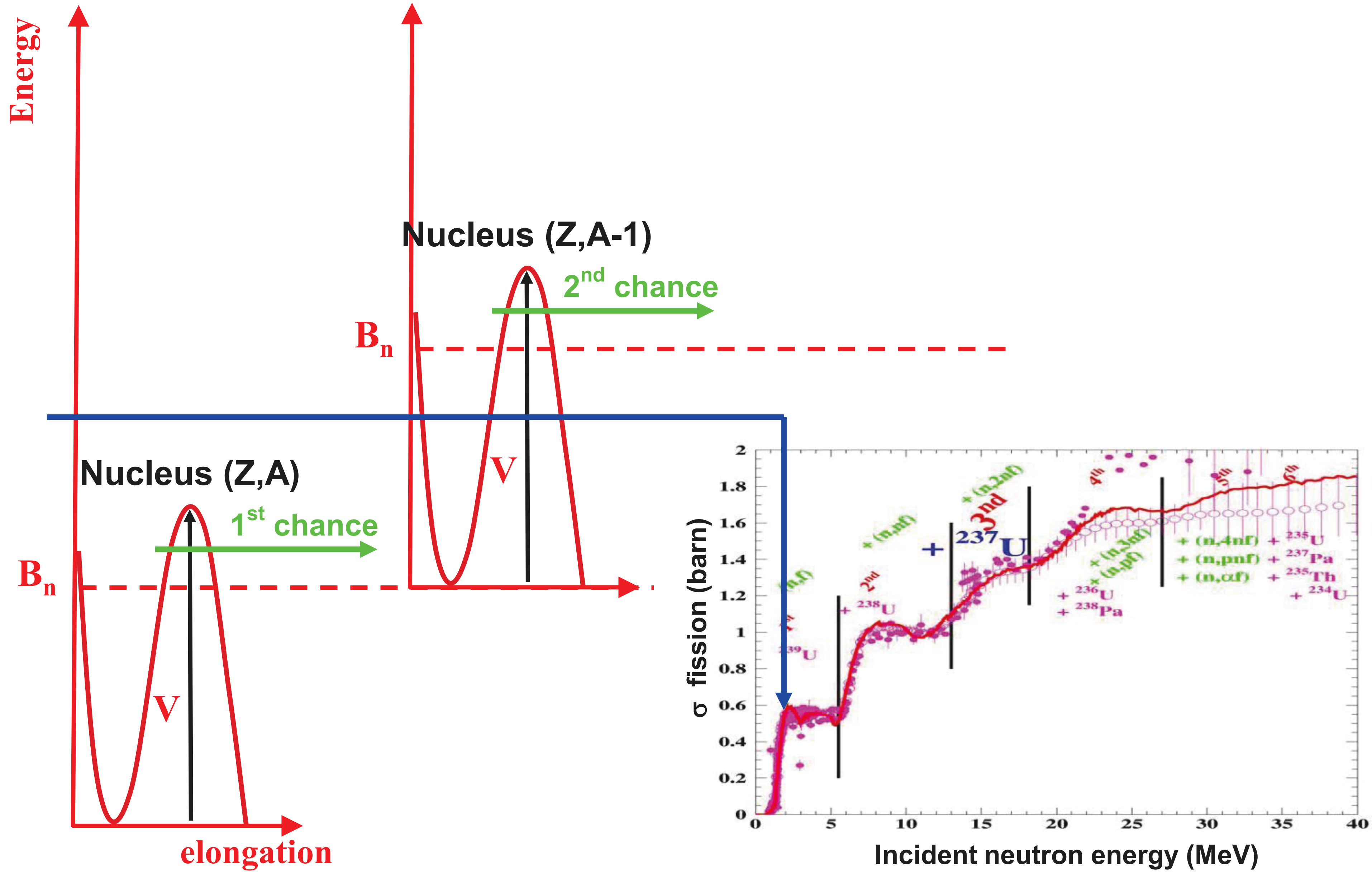

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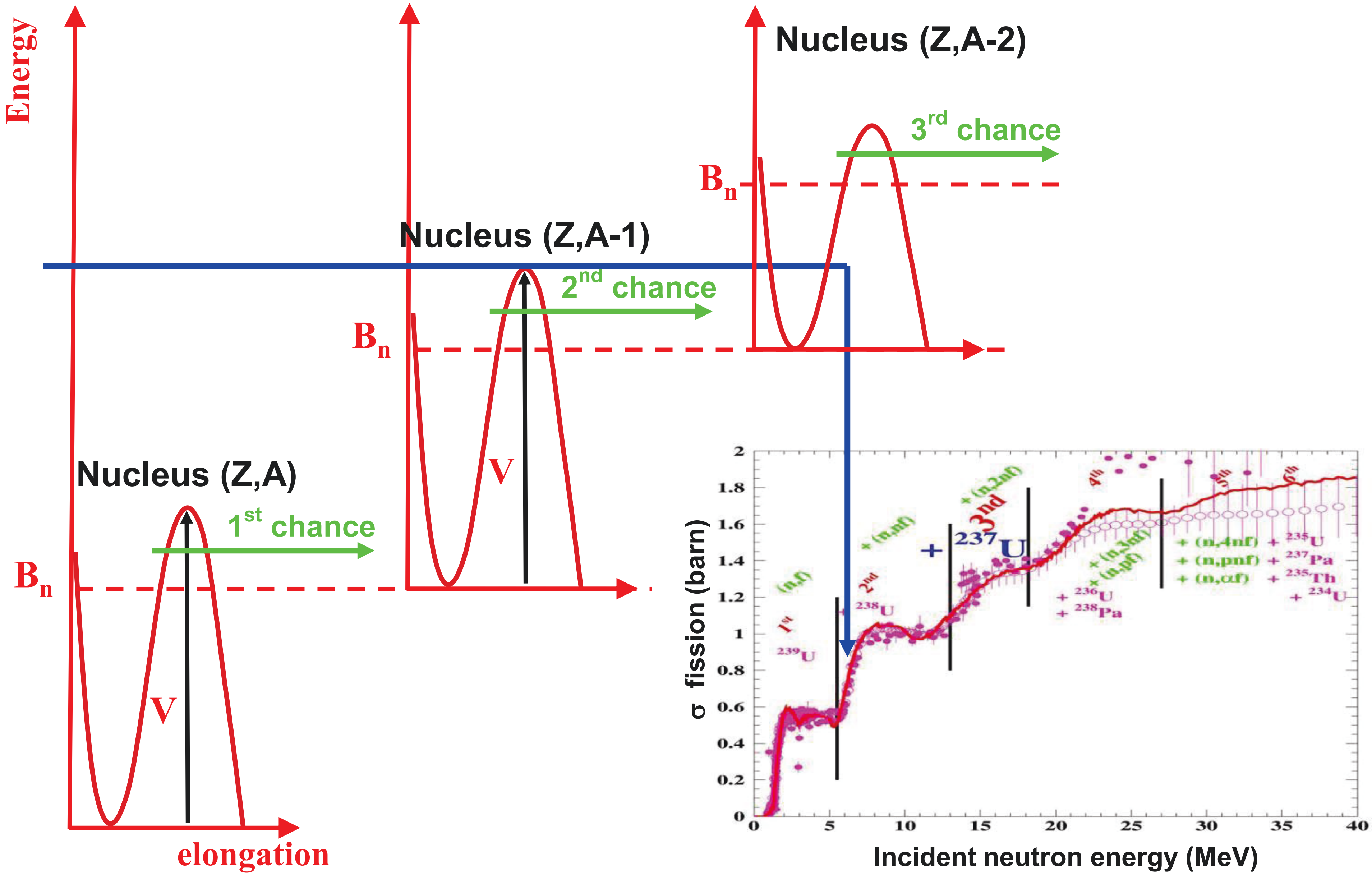

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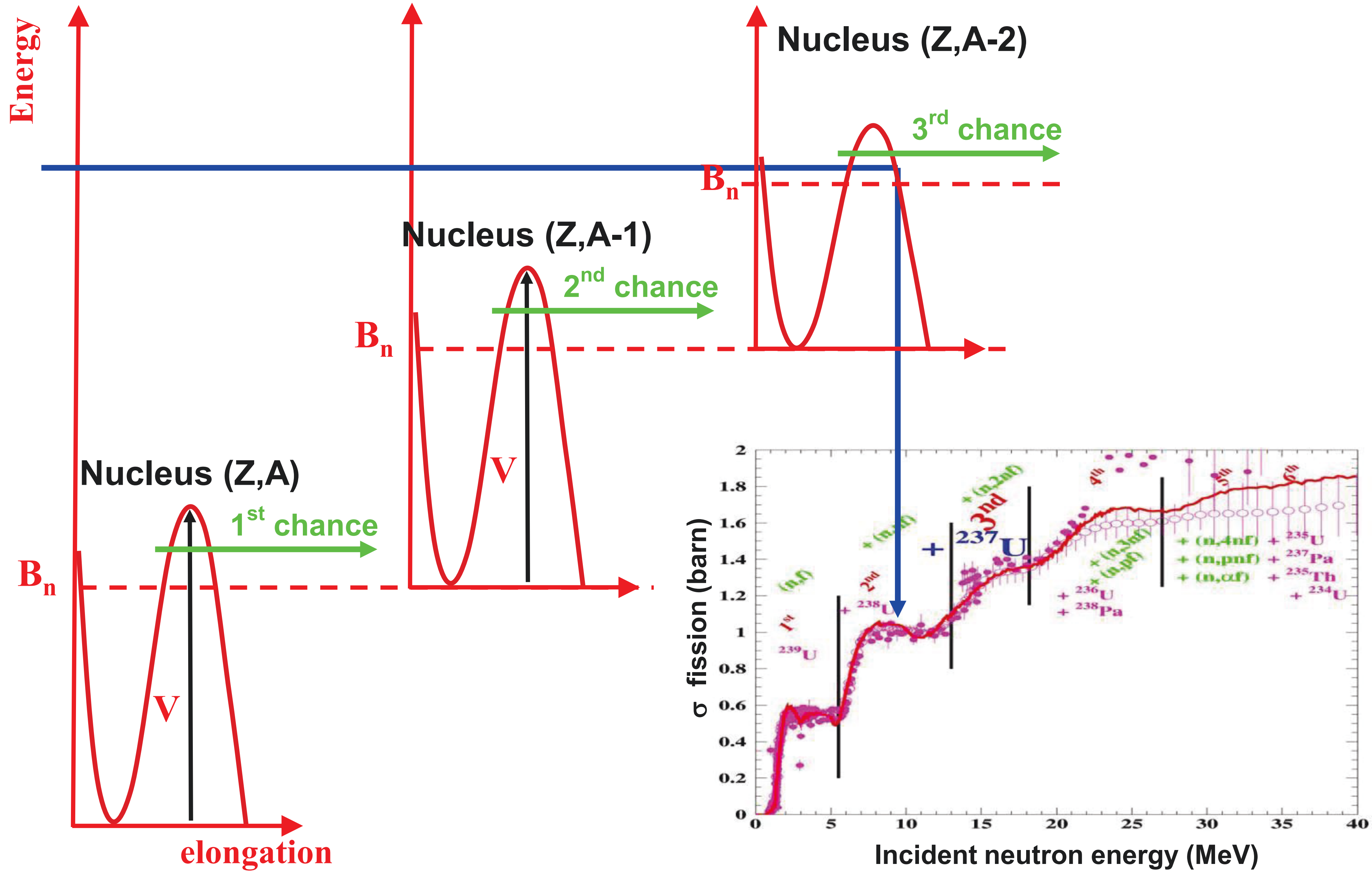

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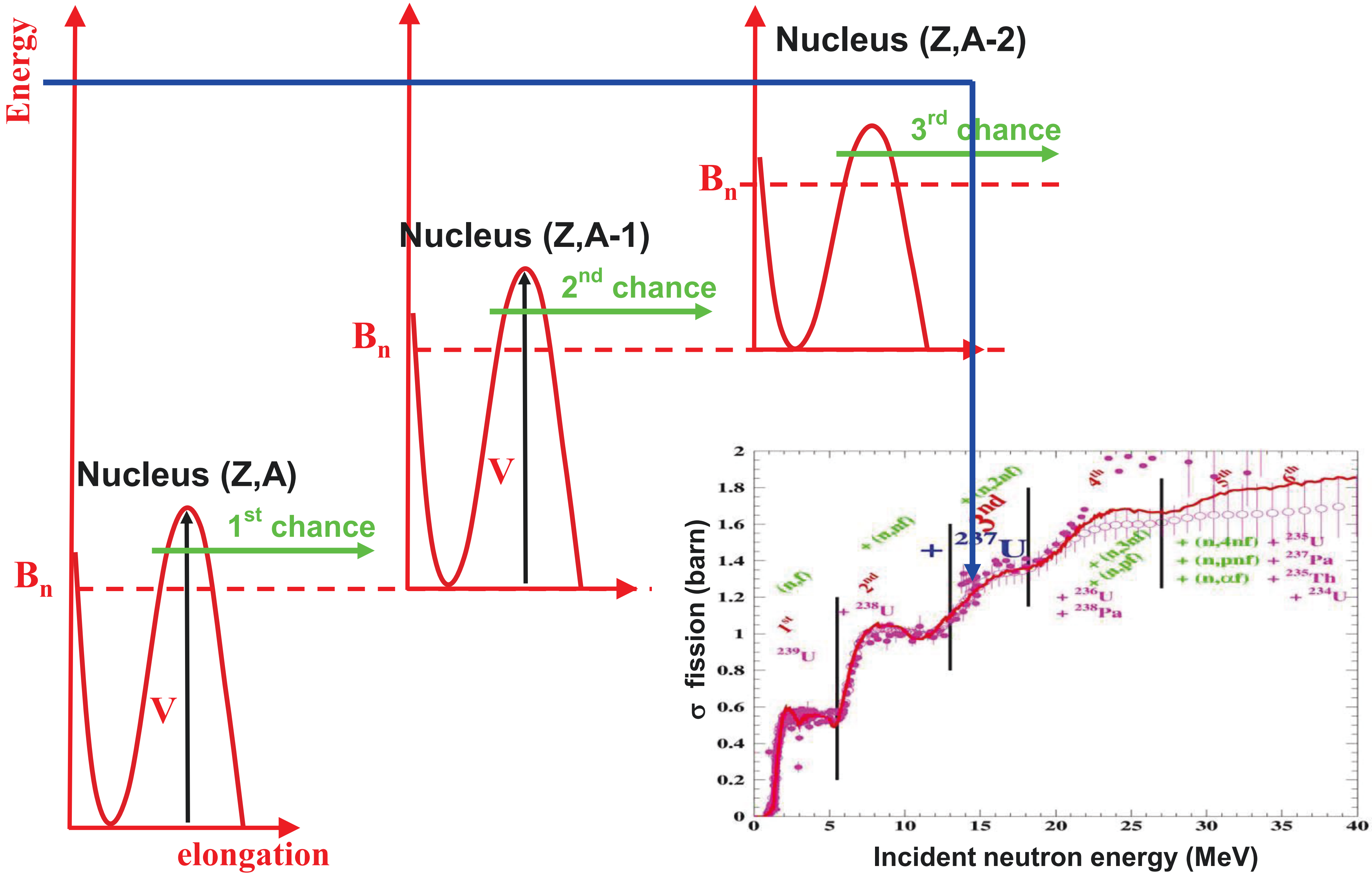
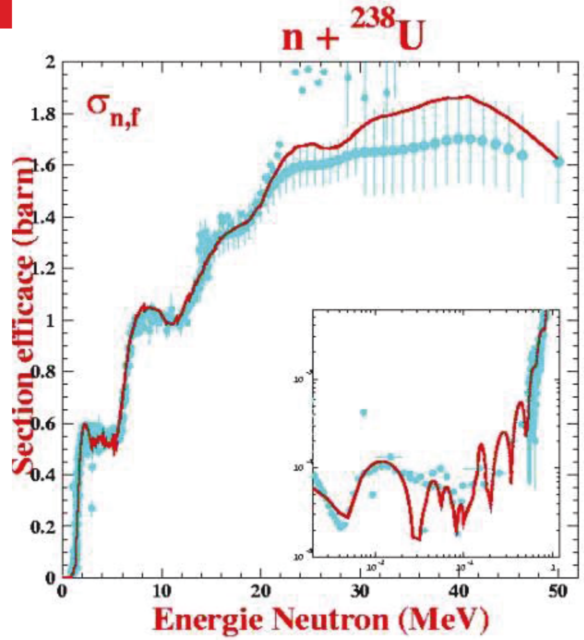


# FINE TUNING AND ACCURACY
## Coherent modeling of fission cross sections (2/3)

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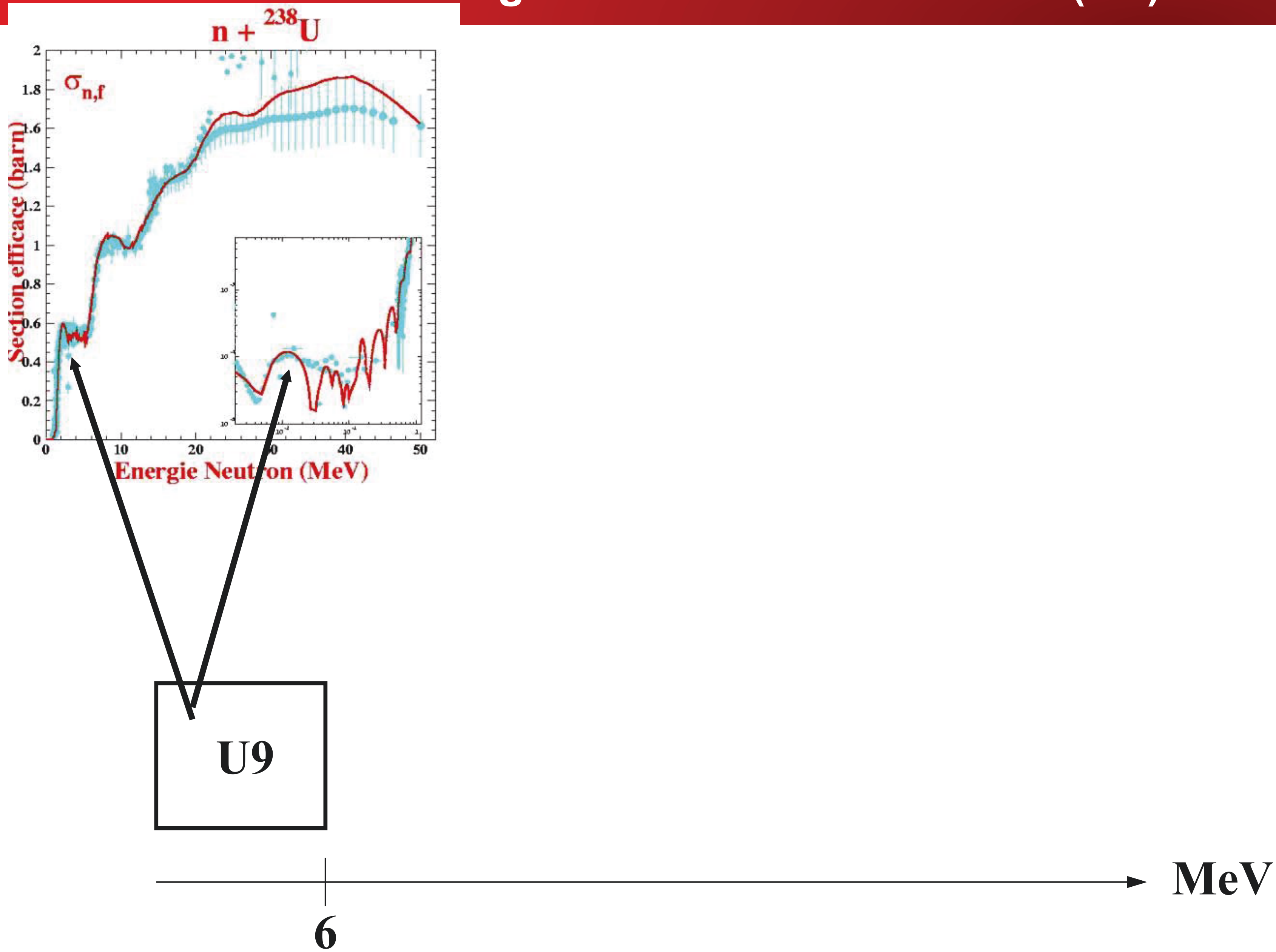

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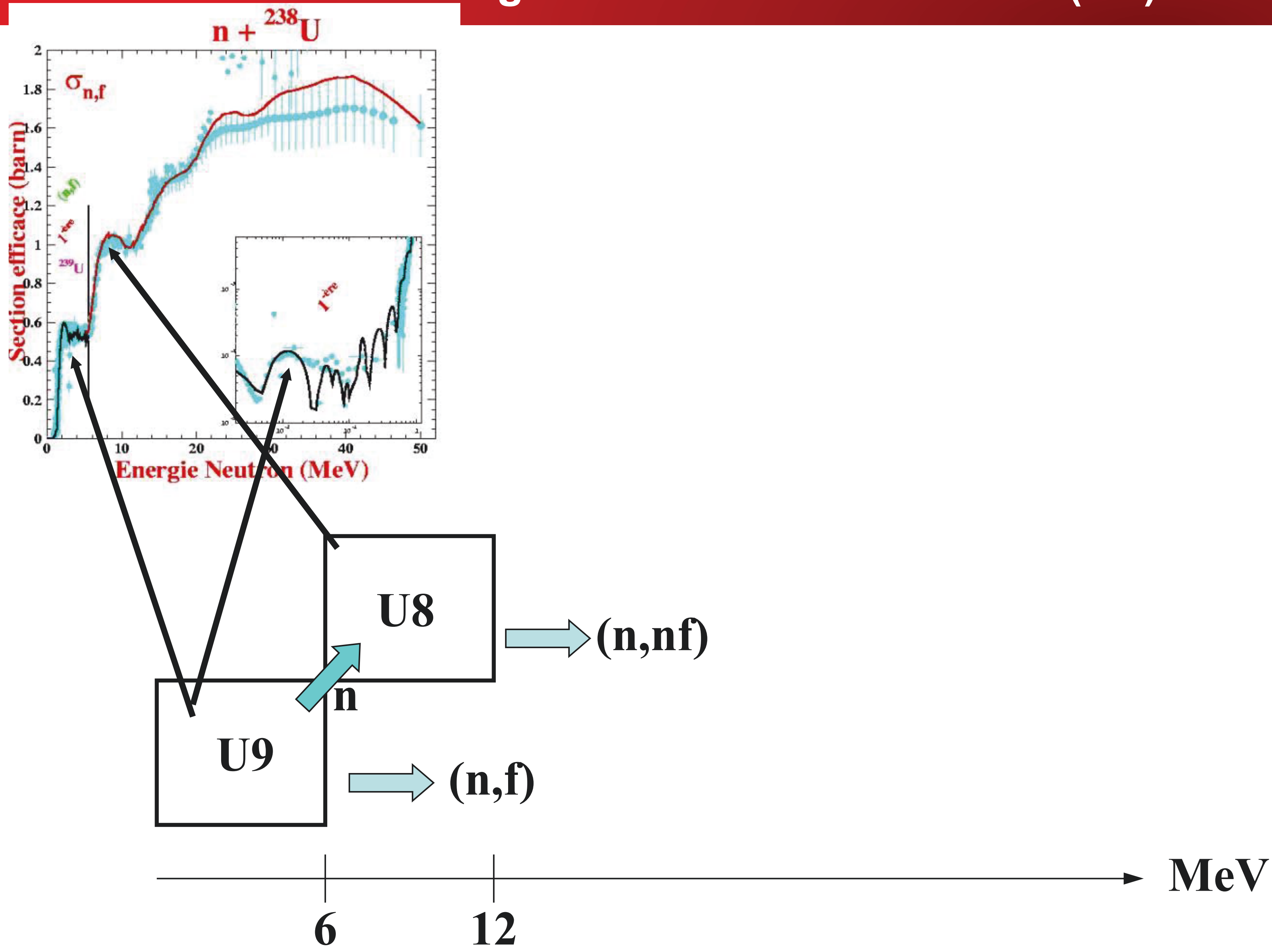

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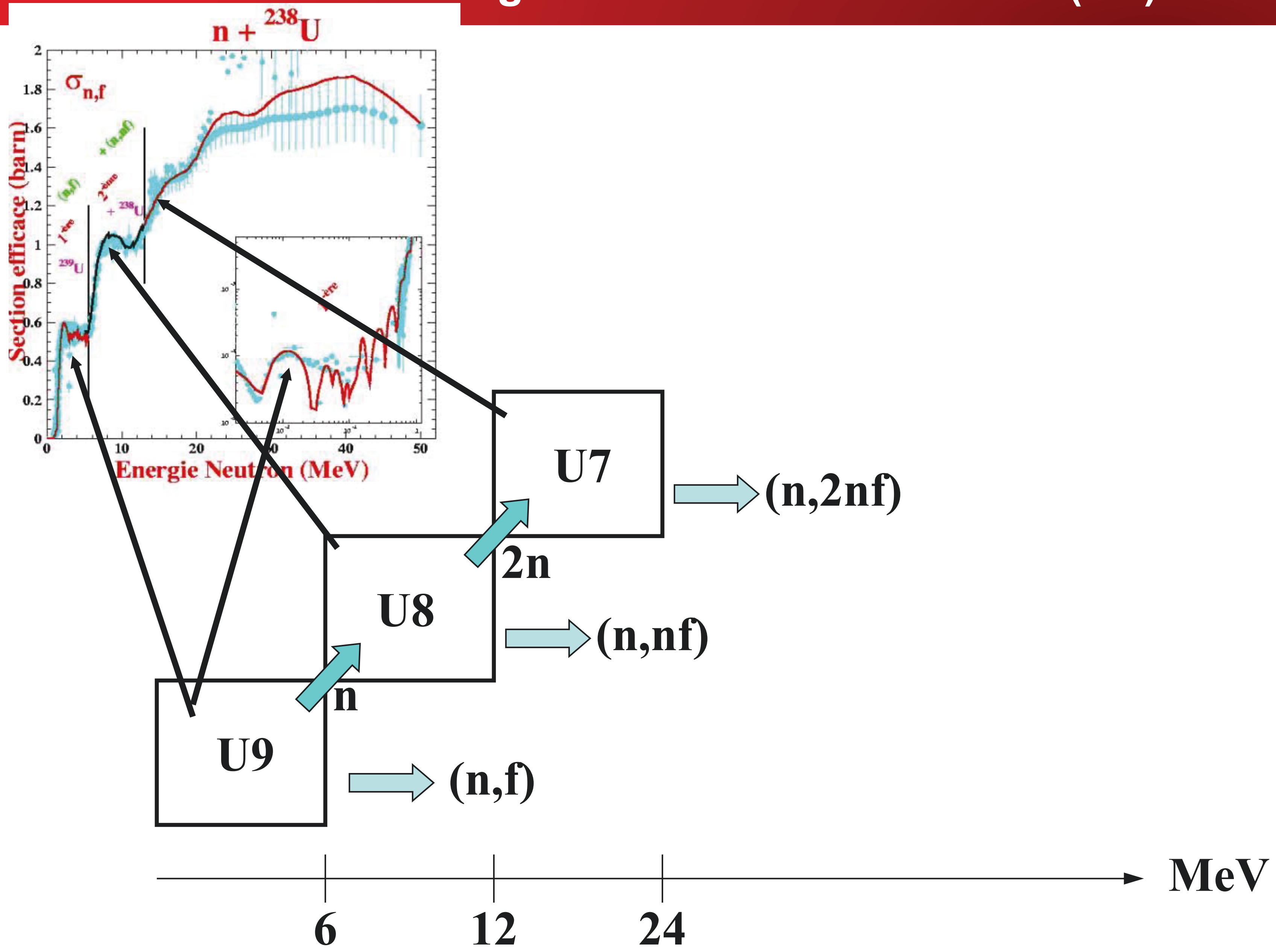

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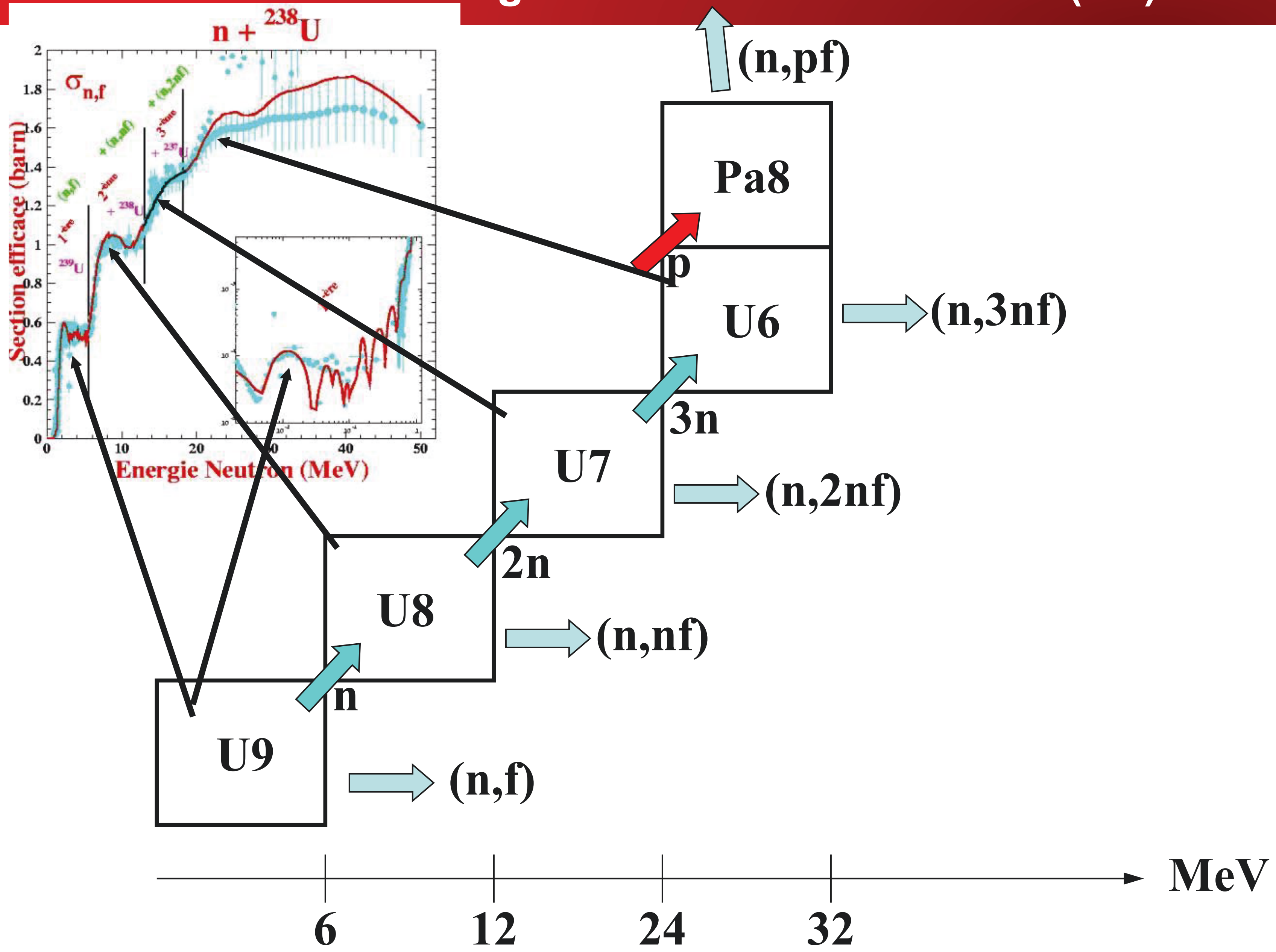

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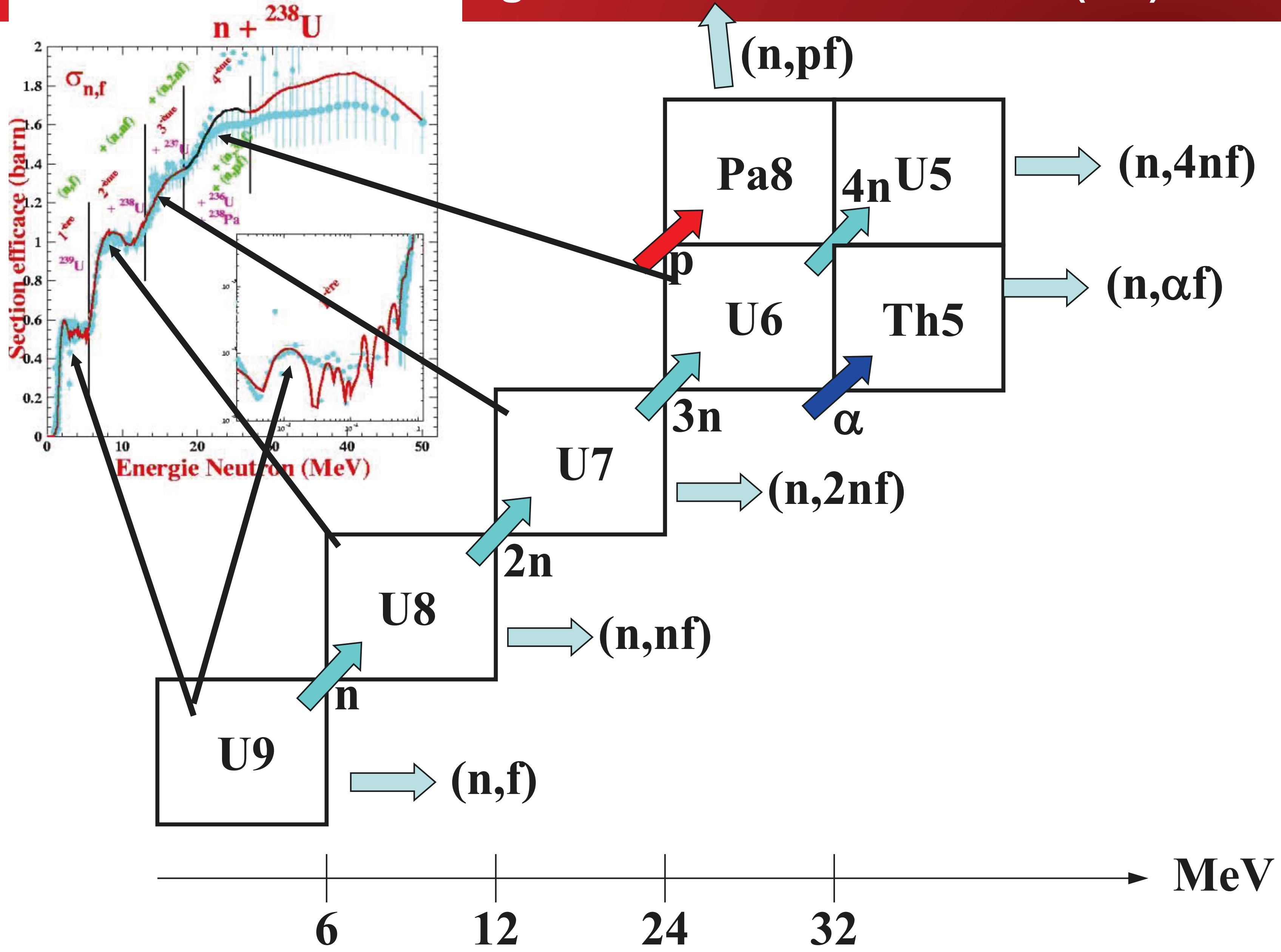

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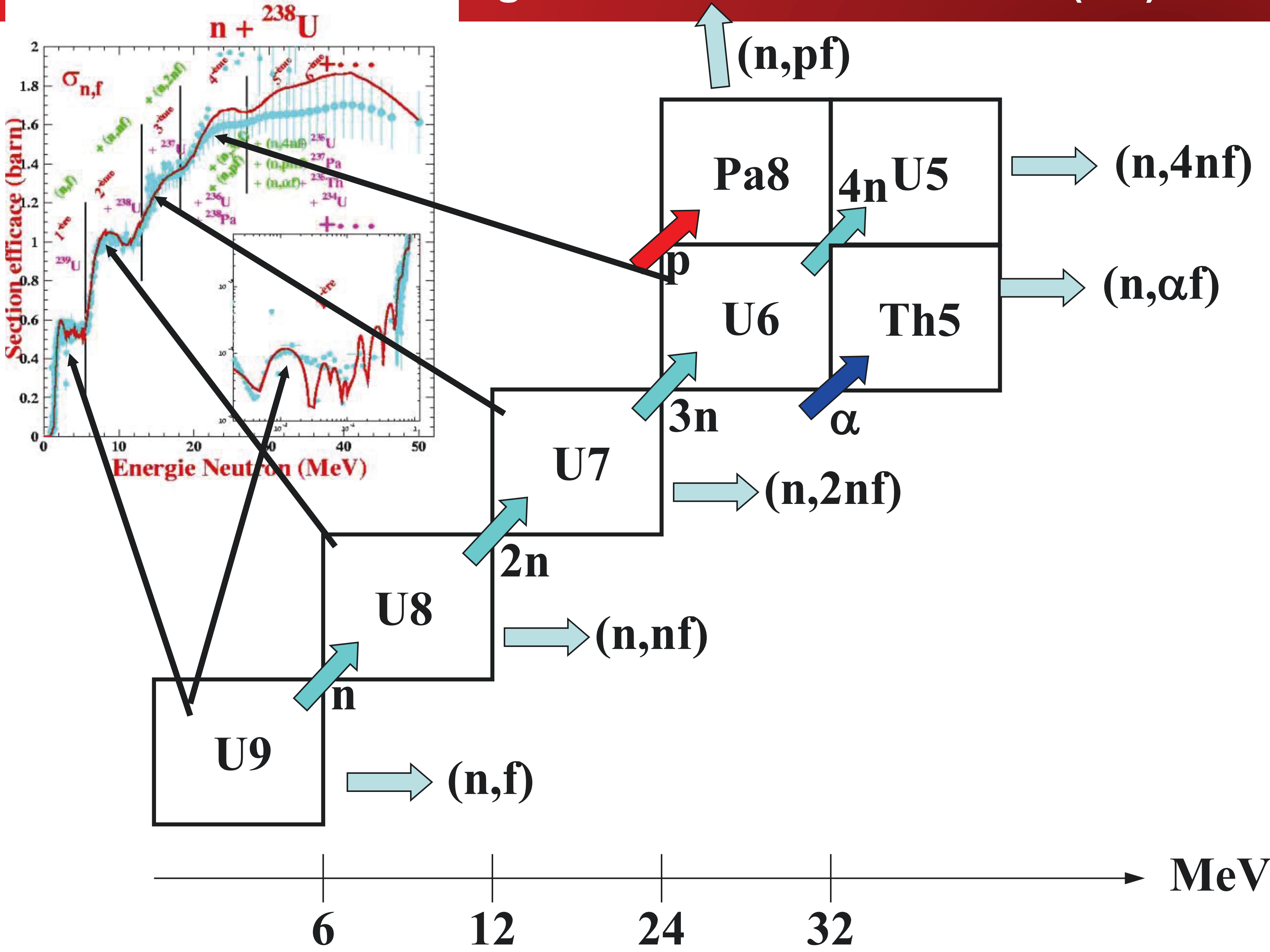

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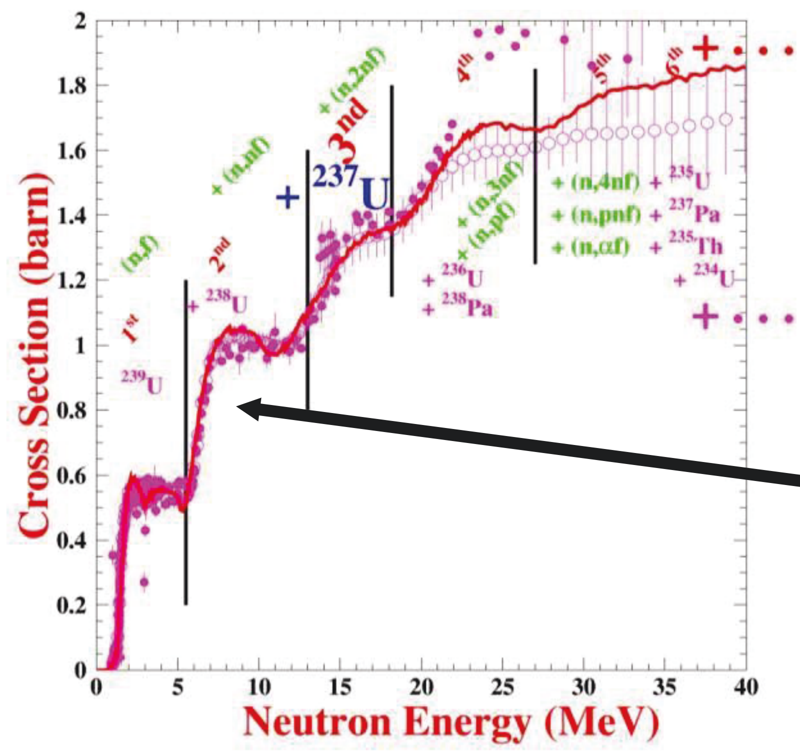
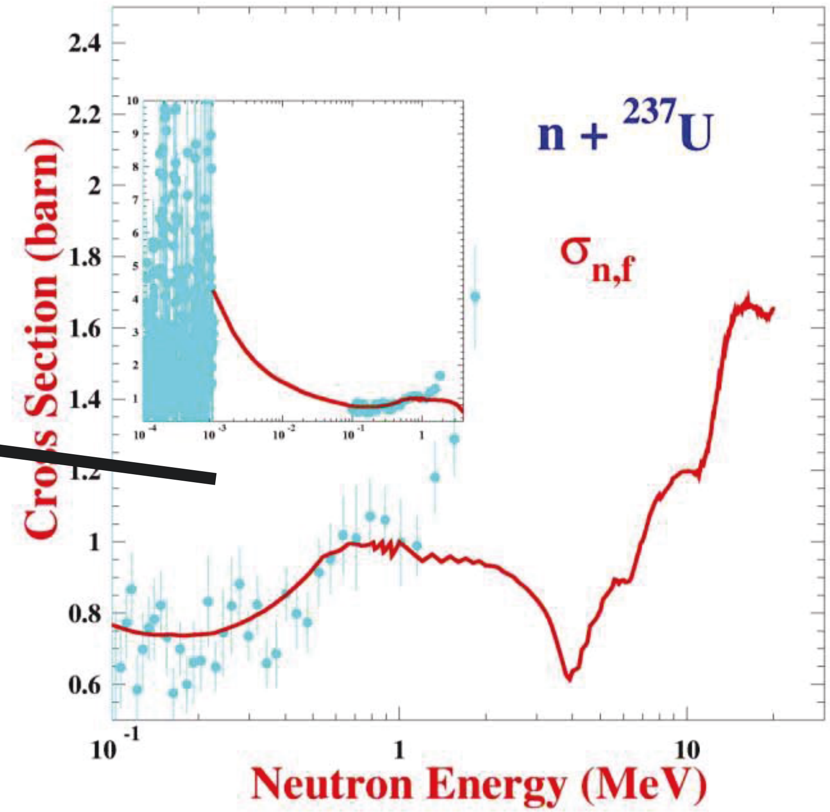
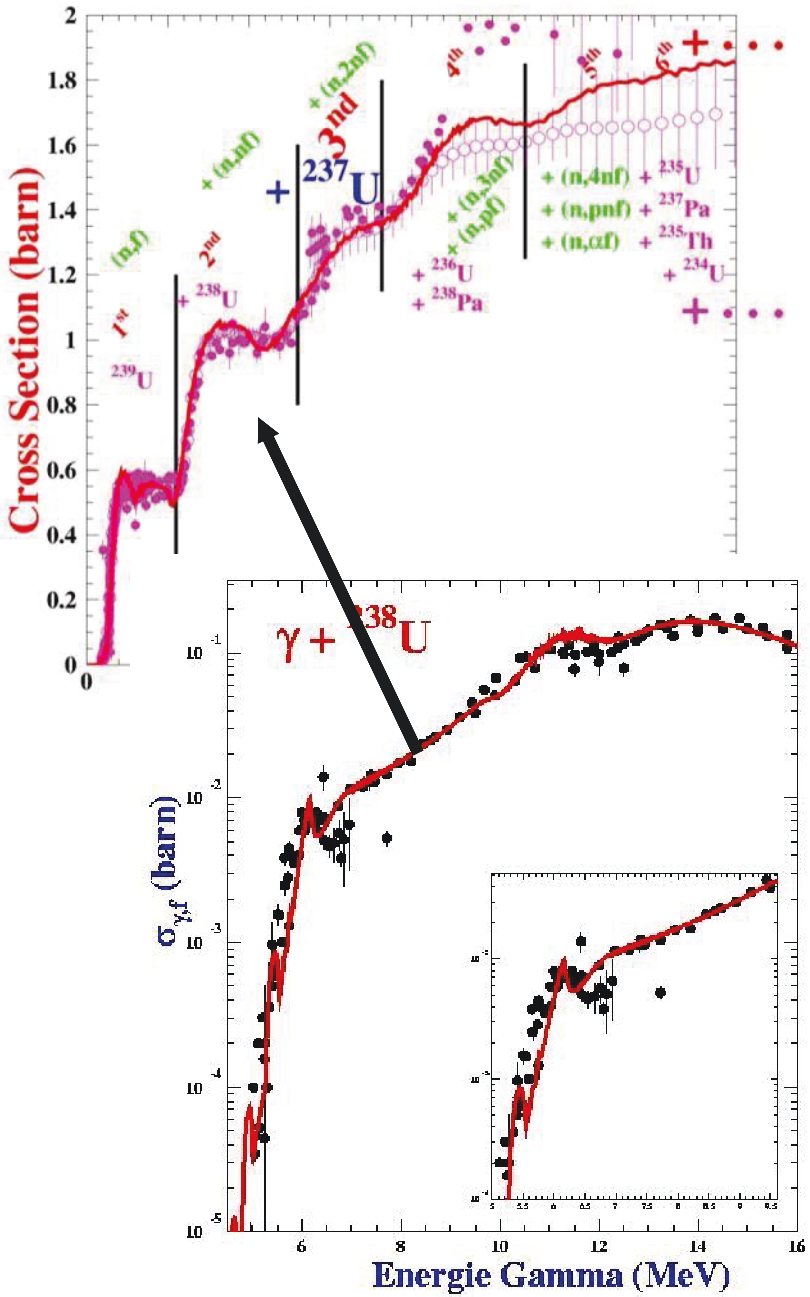
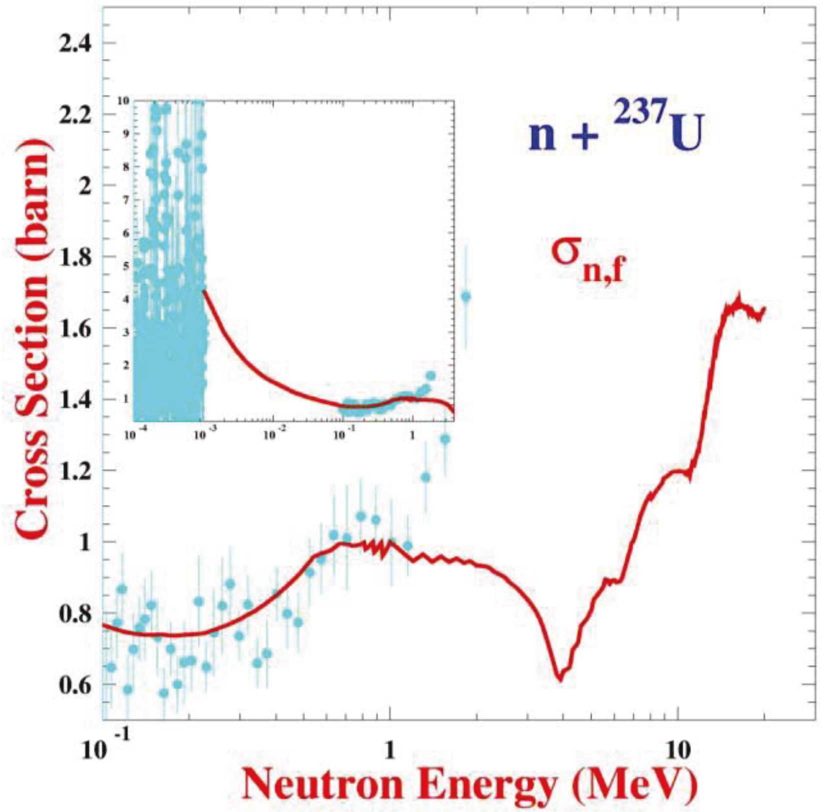


# FINE TUNING AND ACCURACY



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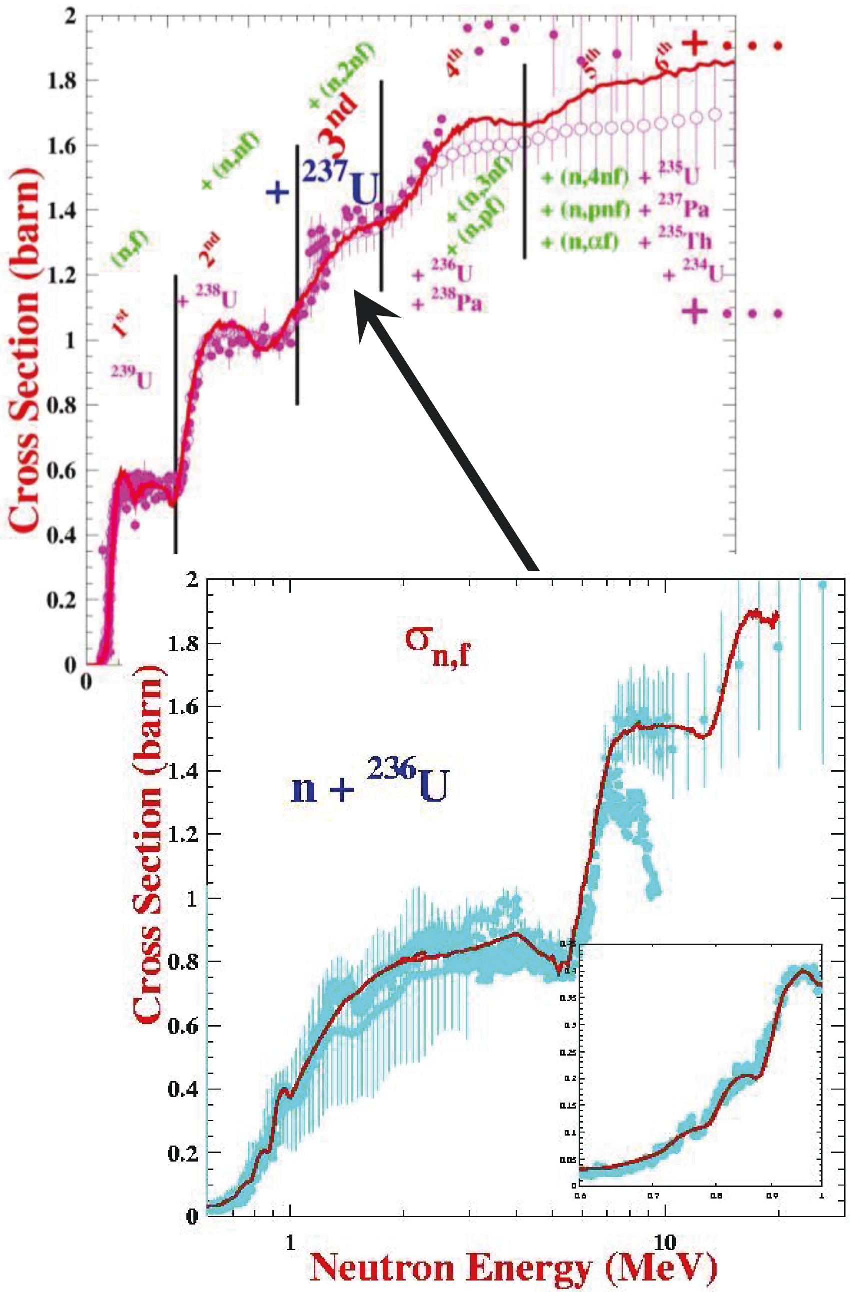


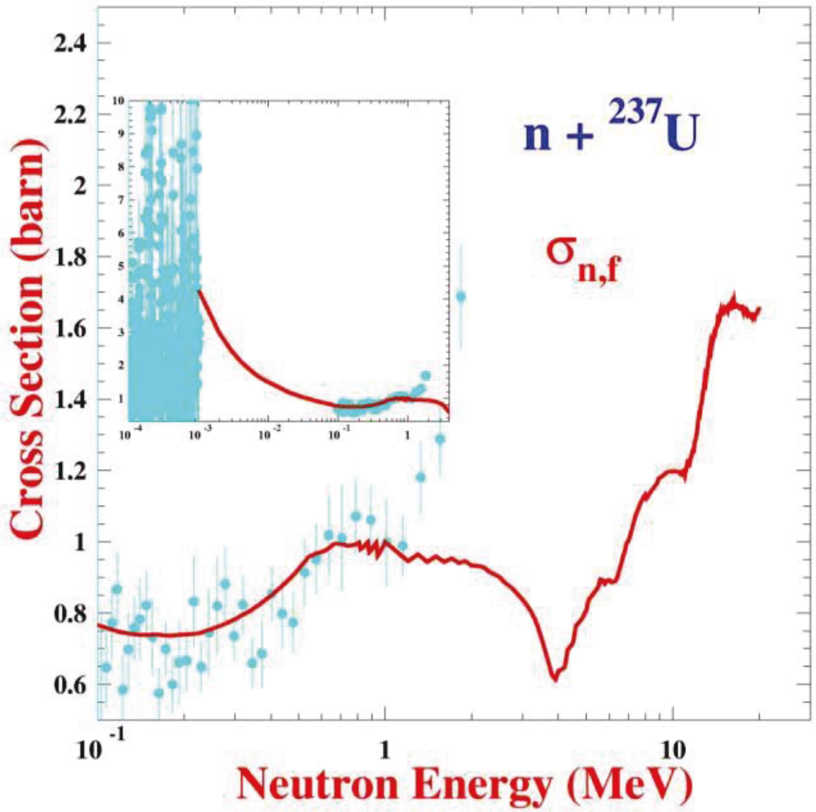

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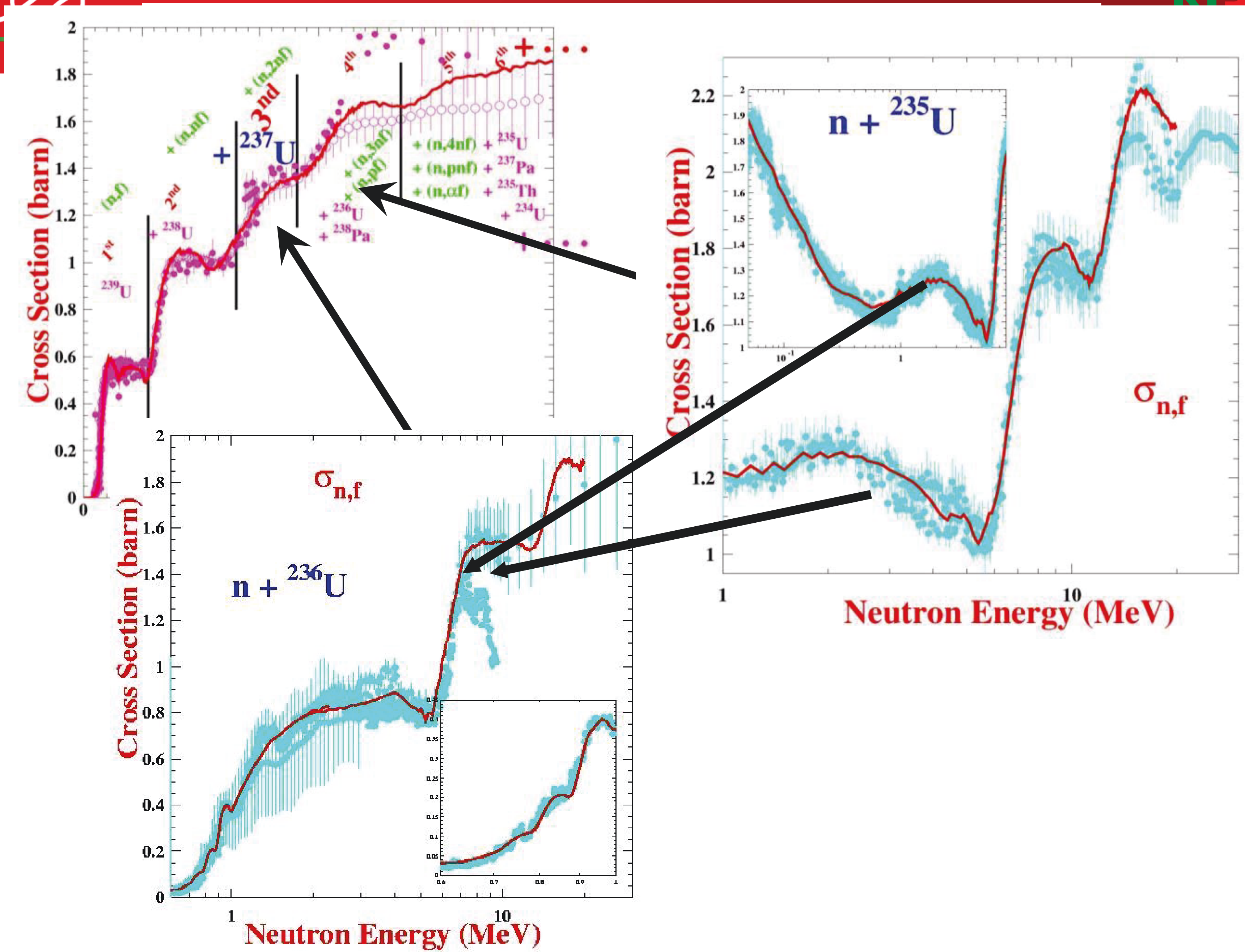

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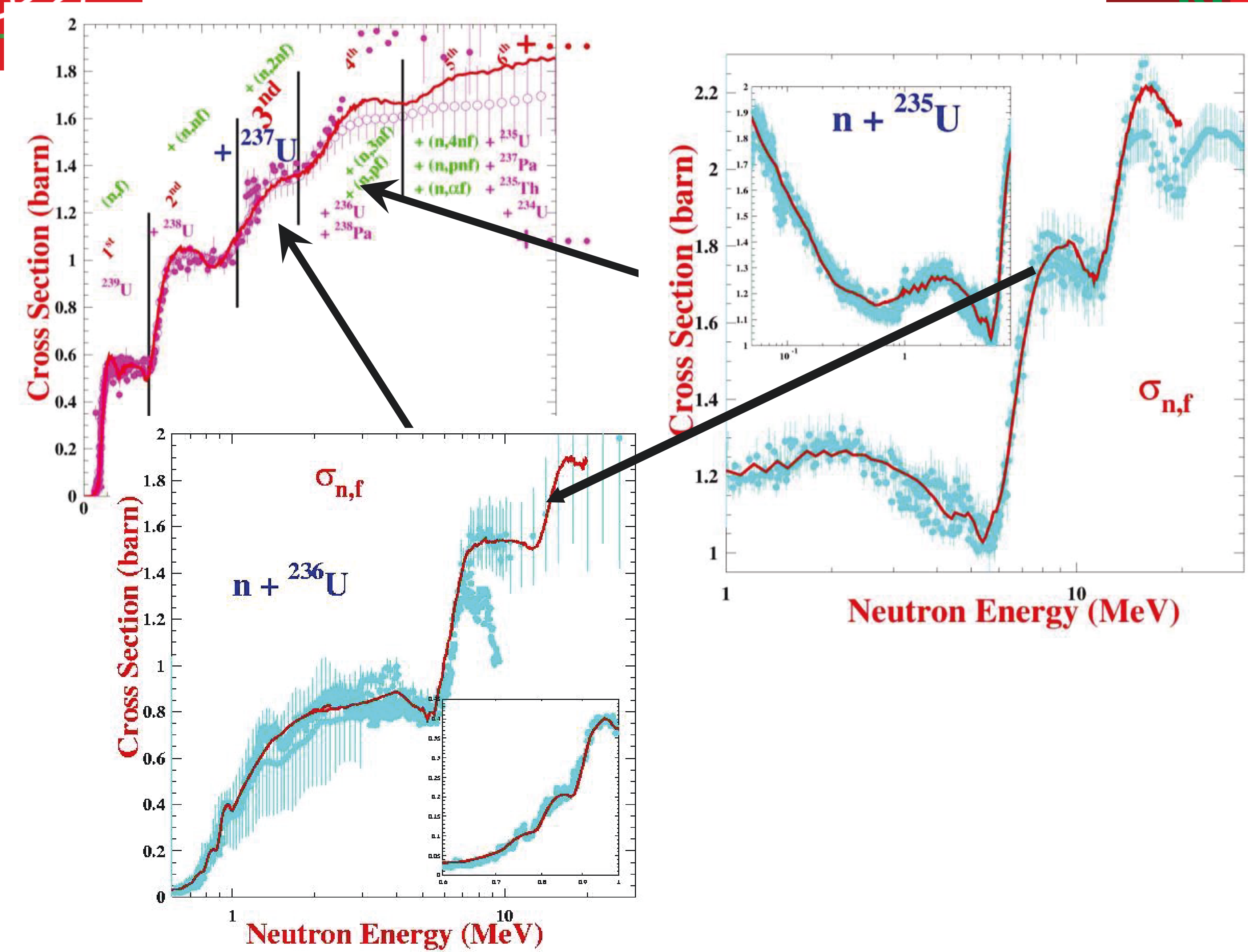
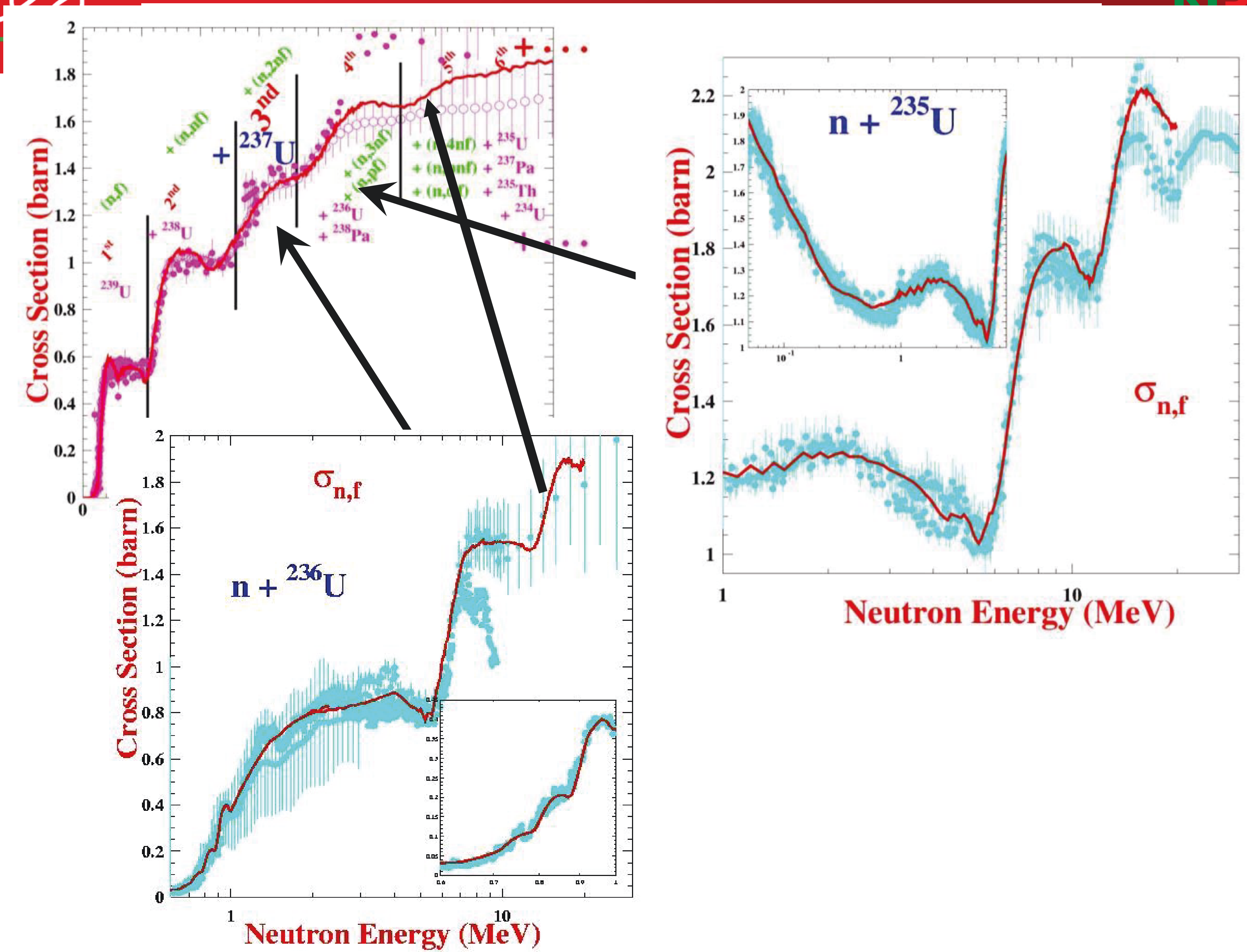
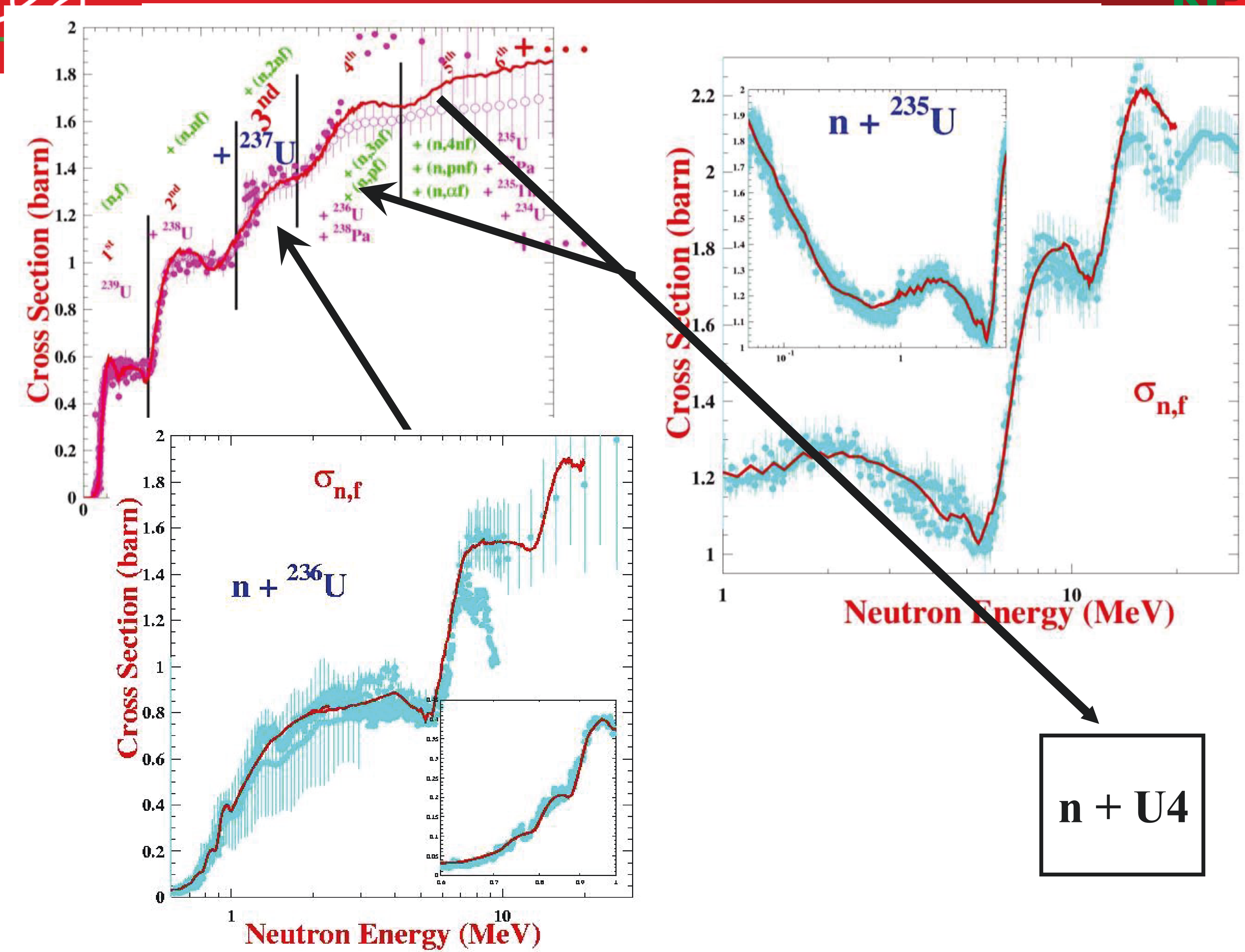


# FINE TUNING AND ACCURACY

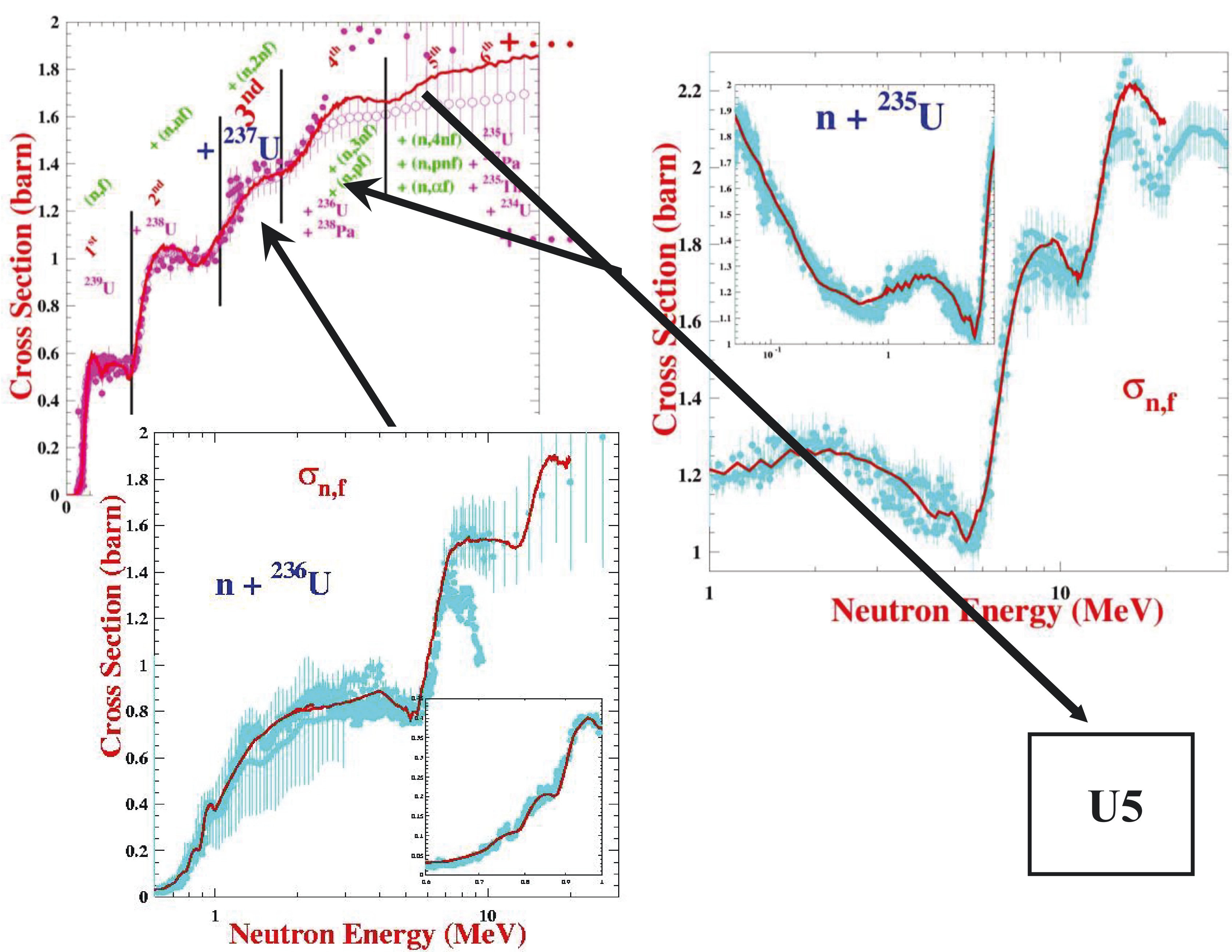


# FINE TUNING AND ACCURACY




n + U4

# FINE TUNING AND ACCURACY



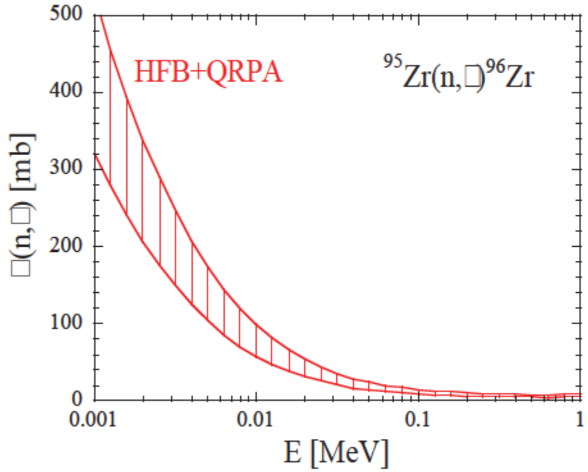
# FINE TUNING AND ACCURACY
## Predictions for unstable target (1/1)

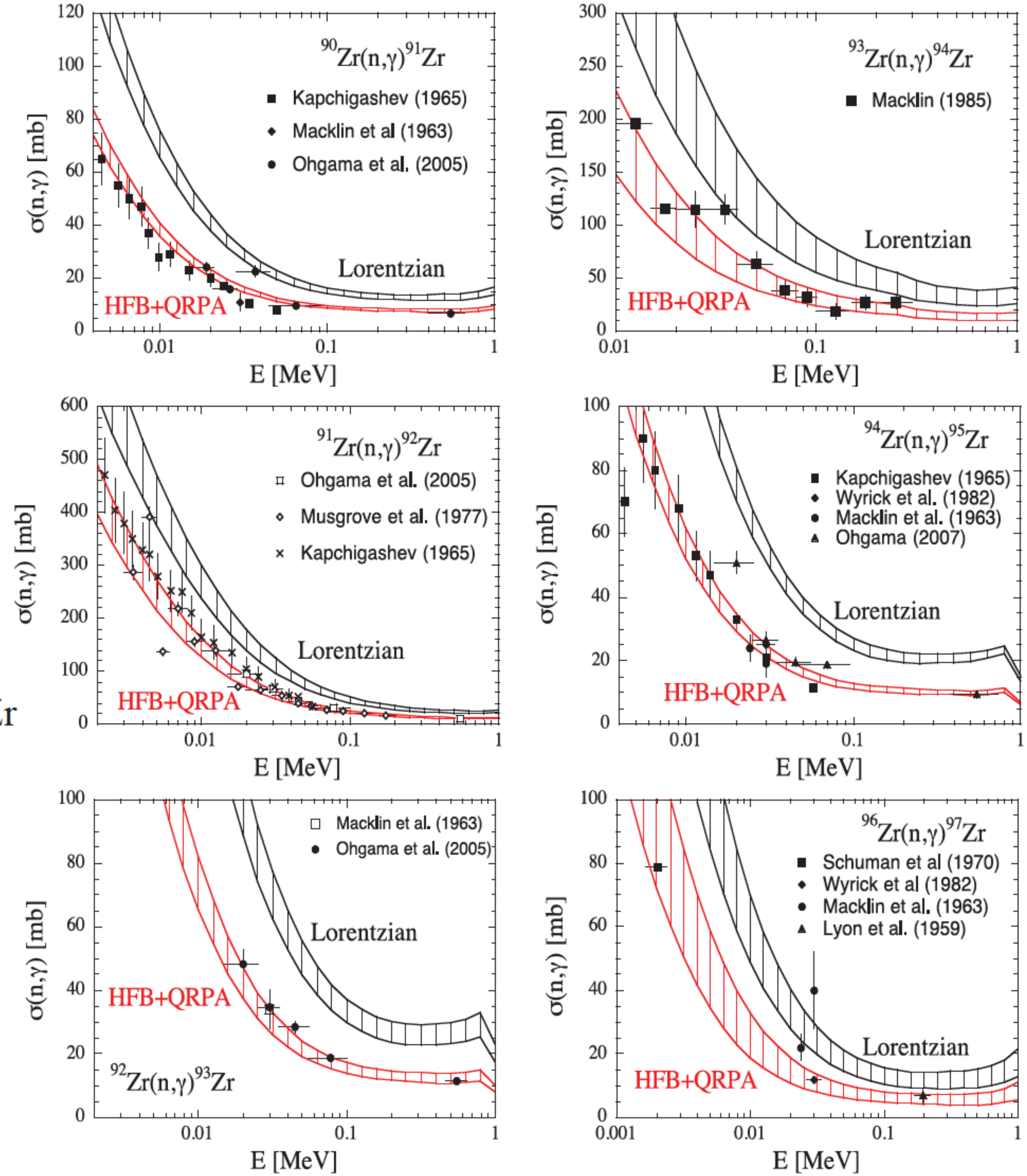
# $^{90-96}$Zr(n,γ) & (γ,n) cross sections

**γ-ray strength constrained on (γ,n) xs**

E1 HFB+QRPA + M1 GR
versus
LORENTZIAN

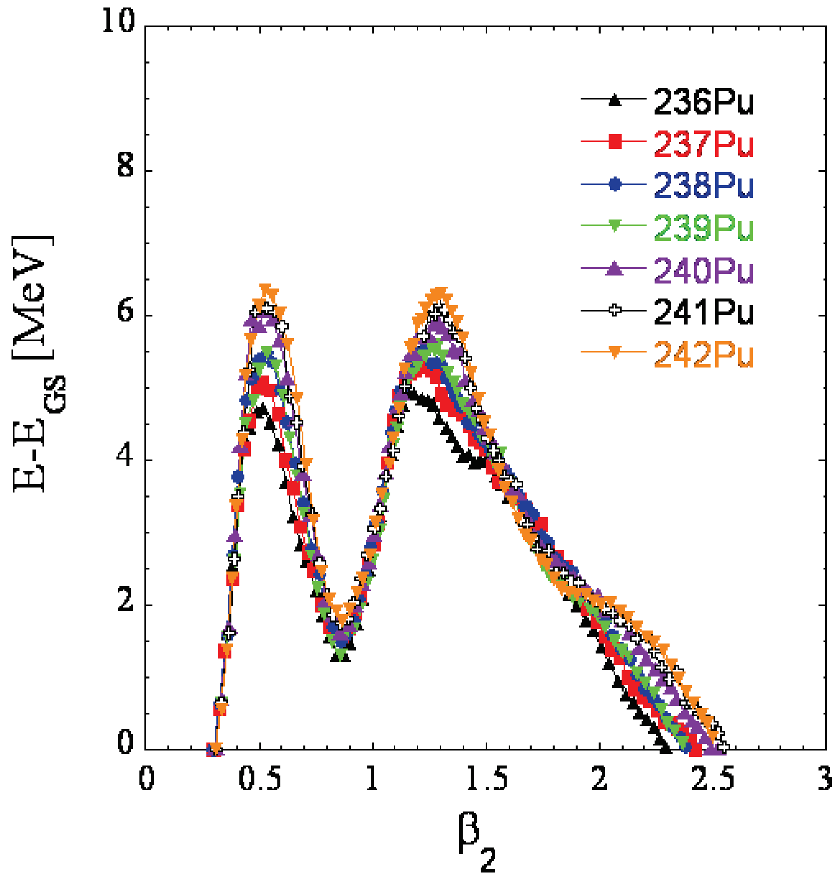
Prediction for short-lived $^{95}$Zr

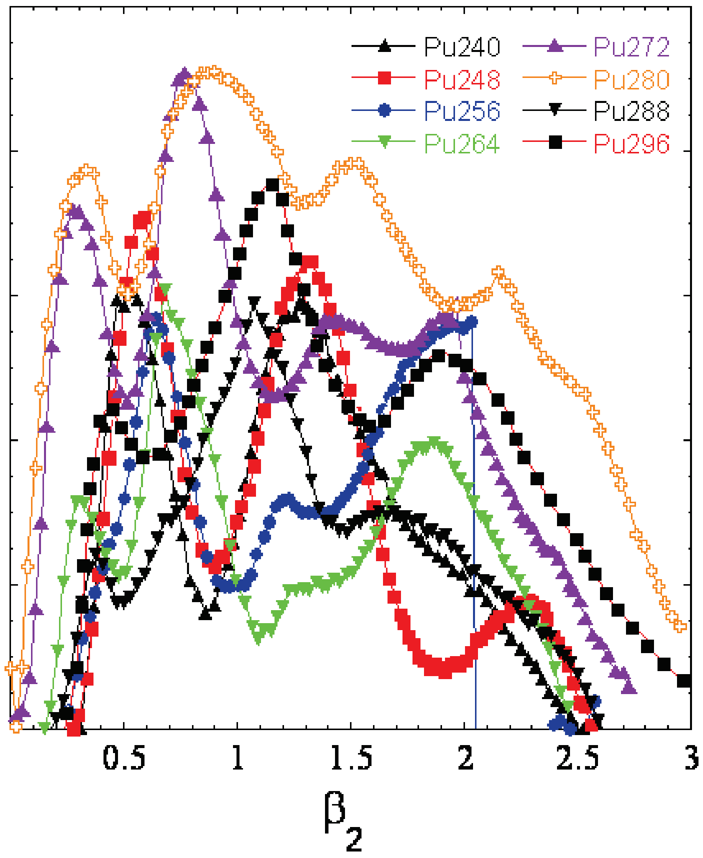


# FINE TUNING AND ACCURACY
## Microscopic modeling of fission cross sections (1/2)

**Microscopic fission barrier shapes**

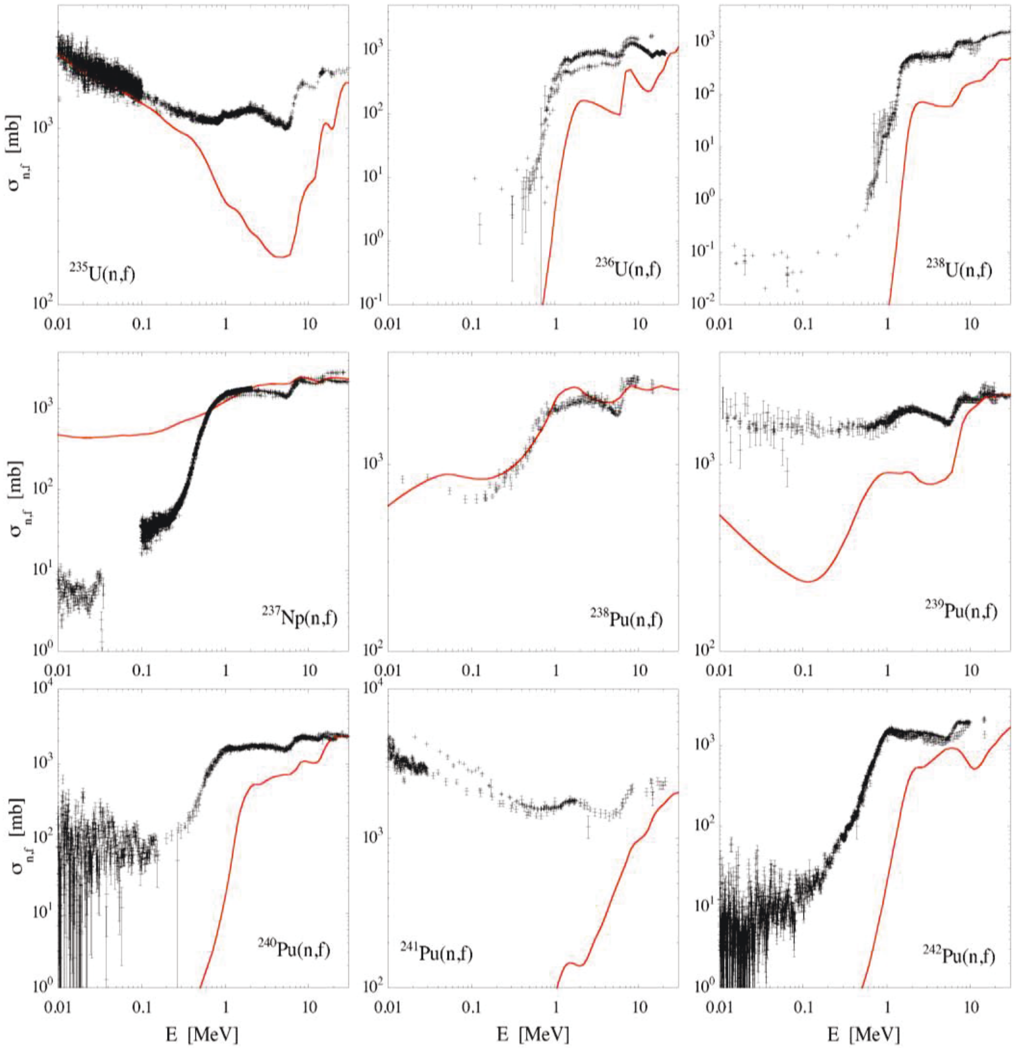



⇒ **For exotic nuclei : strong deviations from Hill-Wheeler.**

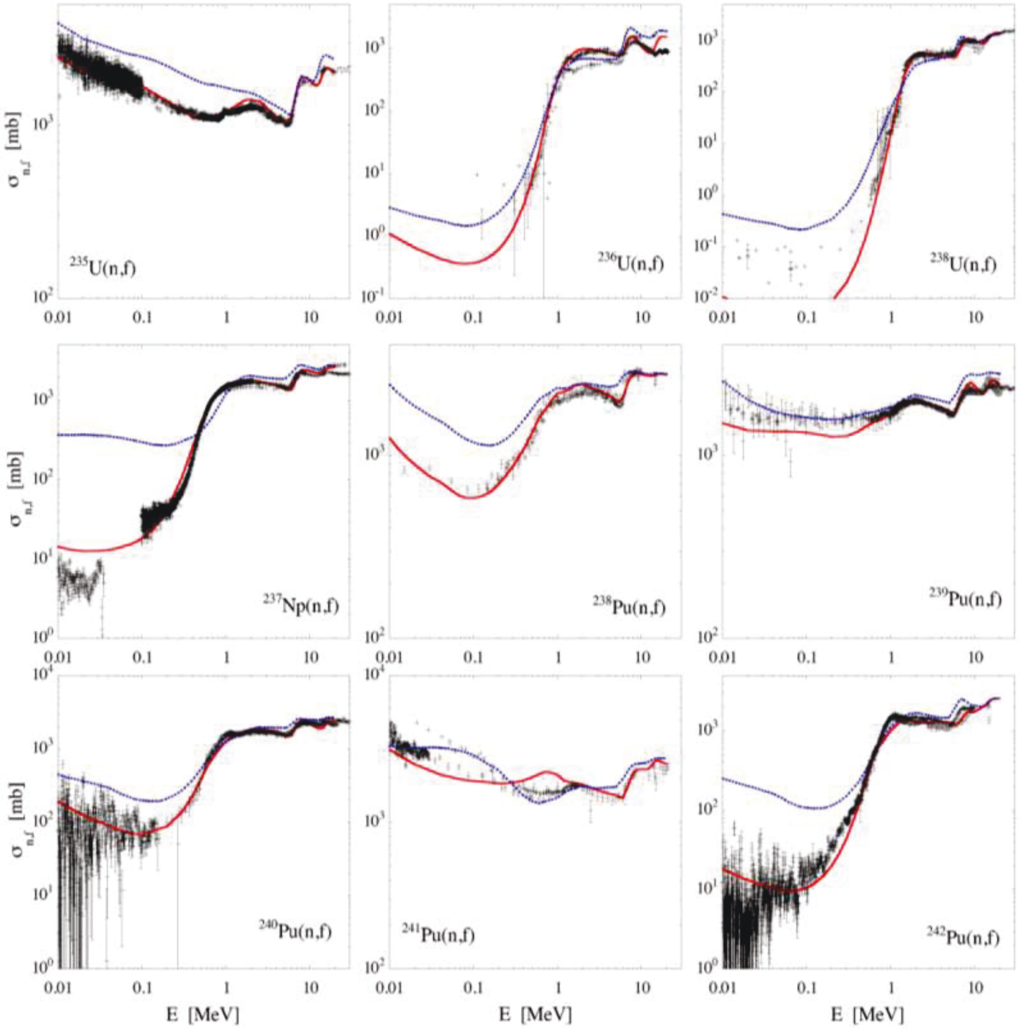
# Microscopic fission cross sections

# FINE TUNING AND ACCURACY
## Microscopic modeling of fission cross sections (2/2)




⇒ **Default calculations not sufficient for applications.**

# FINE TUNING AND ACCURACY
# Microscopic modeling of fission cross sections (2/2)




Fission barriers adjusted for each target

Fission barriers adjusted for each type of target
- odd-odd
- odd-even
- even-odd
- even-even

⇒ **Not ridiculous after few adjustments.**

# FINE TUNING AND ACCURACY
## Coherent microscopic modeling of fission cross sections (1/4)

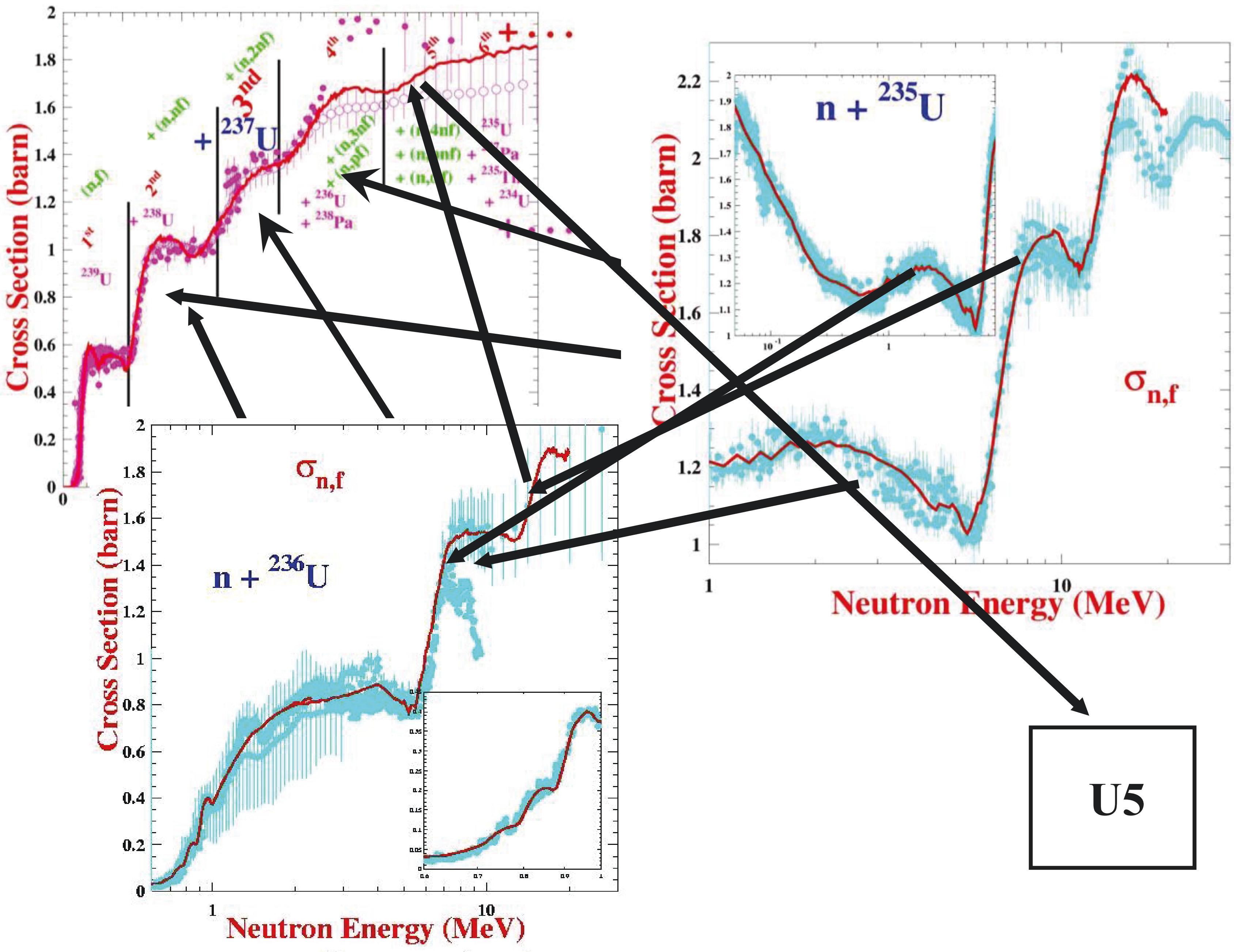
**Coherent fission cross sections with phenomenological approach**

Neutron induced fission on $^{238}U$

- several hundreds of parameters
- unique set for all fission chances or U targets

# FINE TUNING AND ACCURACY

## Coherent microscopic modeling



# Can we do the same with microscopic ingredients ?

# FINE TUNING AND ACCURACY
## Coherent microscopic modeling of fission cross sections (3/4)

**HFB-14 predictions of fission barriers and NLD at saddle points**, including renormalization (max 5 parameters) of

- fission path height: $B_f'(\beta_2) = B_f(\beta_2) \times v_{corr}$
- NLD at 1st and 2d saddle points:

$$\rho'(U,J,P) = \rho(U-\delta,J,P)e^{\alpha\sqrt{U-\delta}}$$

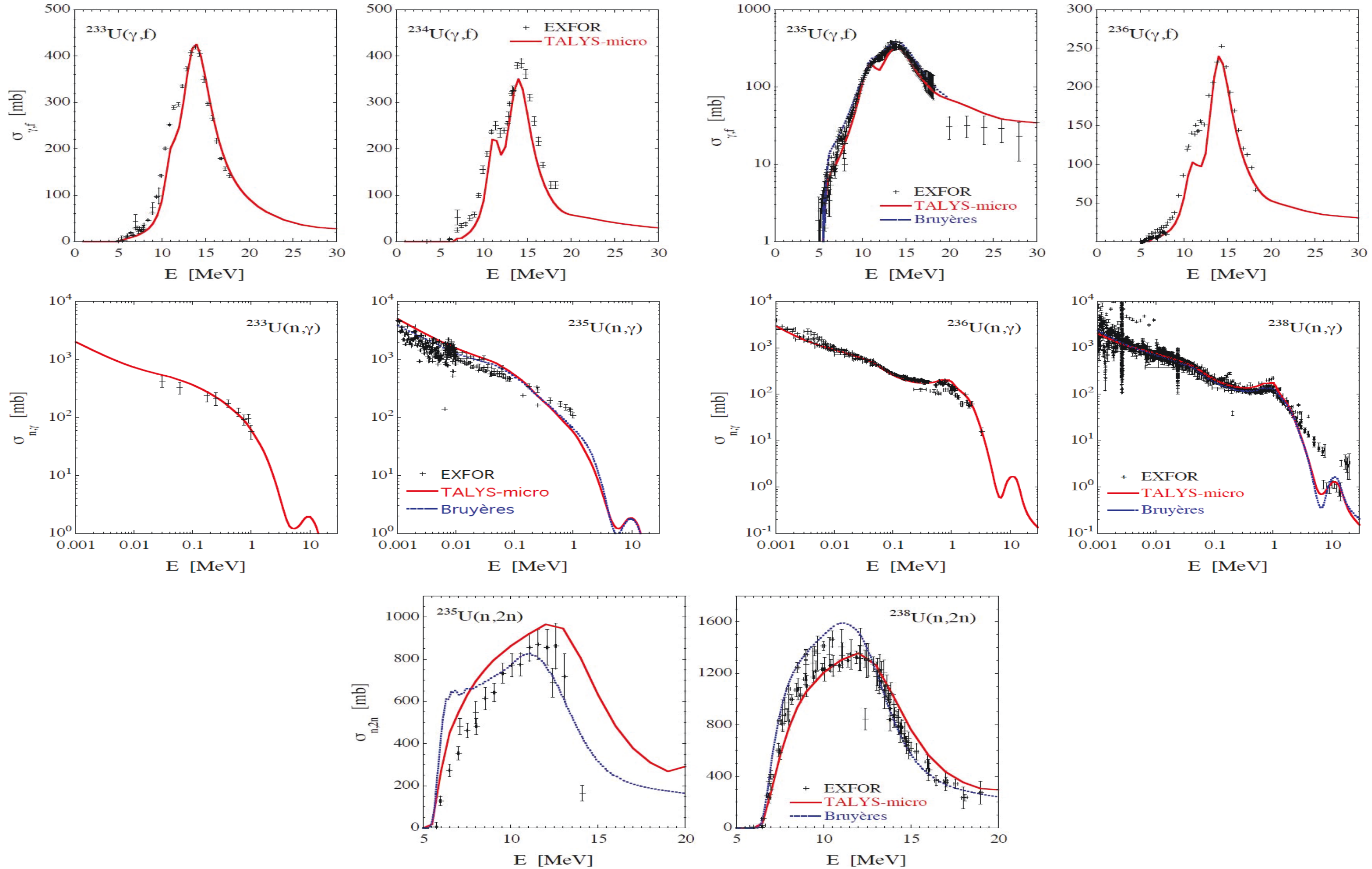
**Additional nuclear inputs:**

- Nuclear structure properties: HFB-14 (Goriely et al. 2007)
- Optical potential: Soukhovitskii et al. (2004)
- $\gamma$-ray strength: Hybrid model (Goriely, 1998)
- NLD: HFB-14 plus combinatorial model (Goriely et al., 2008) normalized on s-wave spacings and discrete excited levels

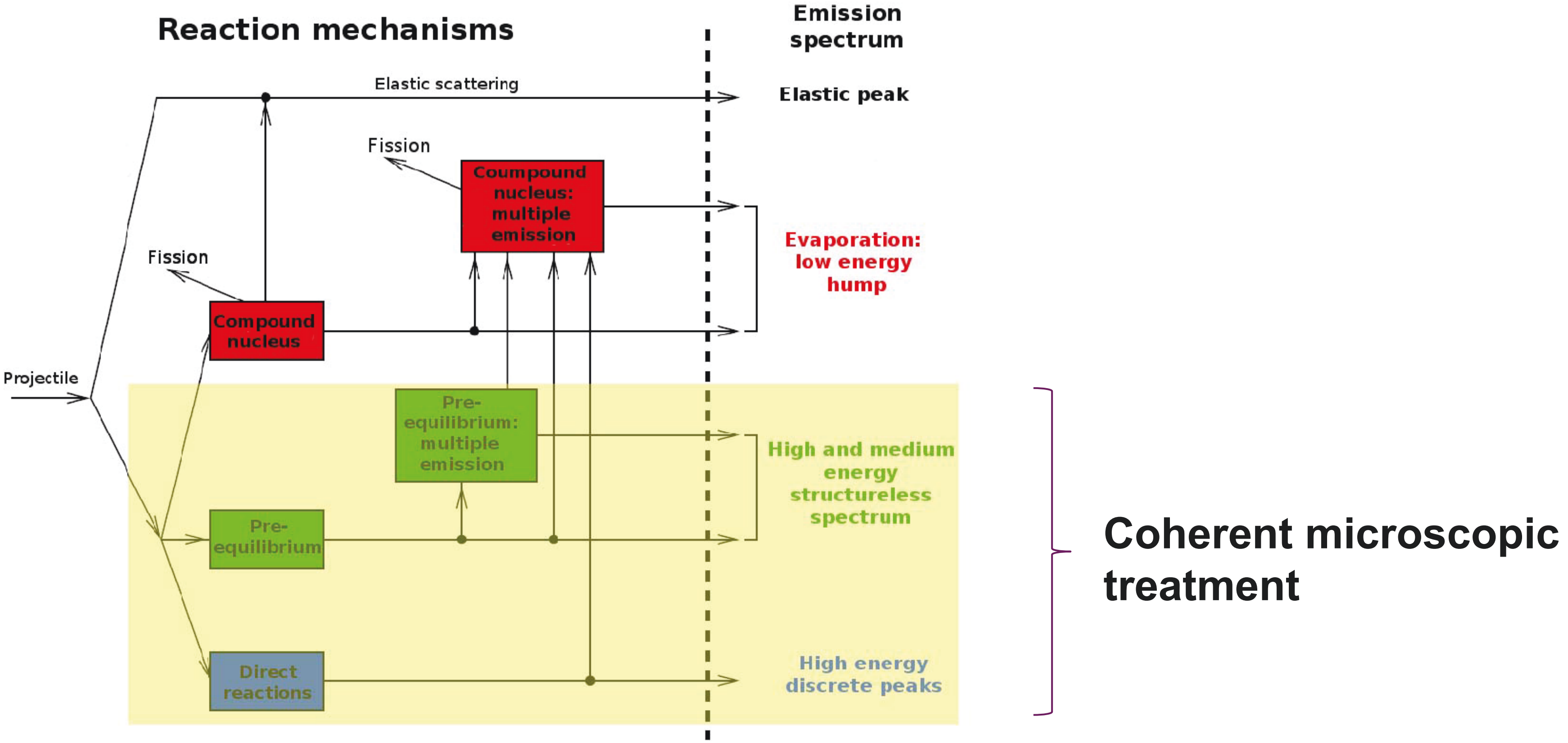
**Note:**

- 1 UNIQUE set of nuclear ingredients for all U isotopes
- no class 2 states included
- no discrete transition states included

# FINE TUNING AND ACCURACY
## Coherent microscopic modeling of fission cross sections (4/4)



# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (1/5)




**Spherical nuclei**

⇒ **Microscopic structure from RPA (easy)**

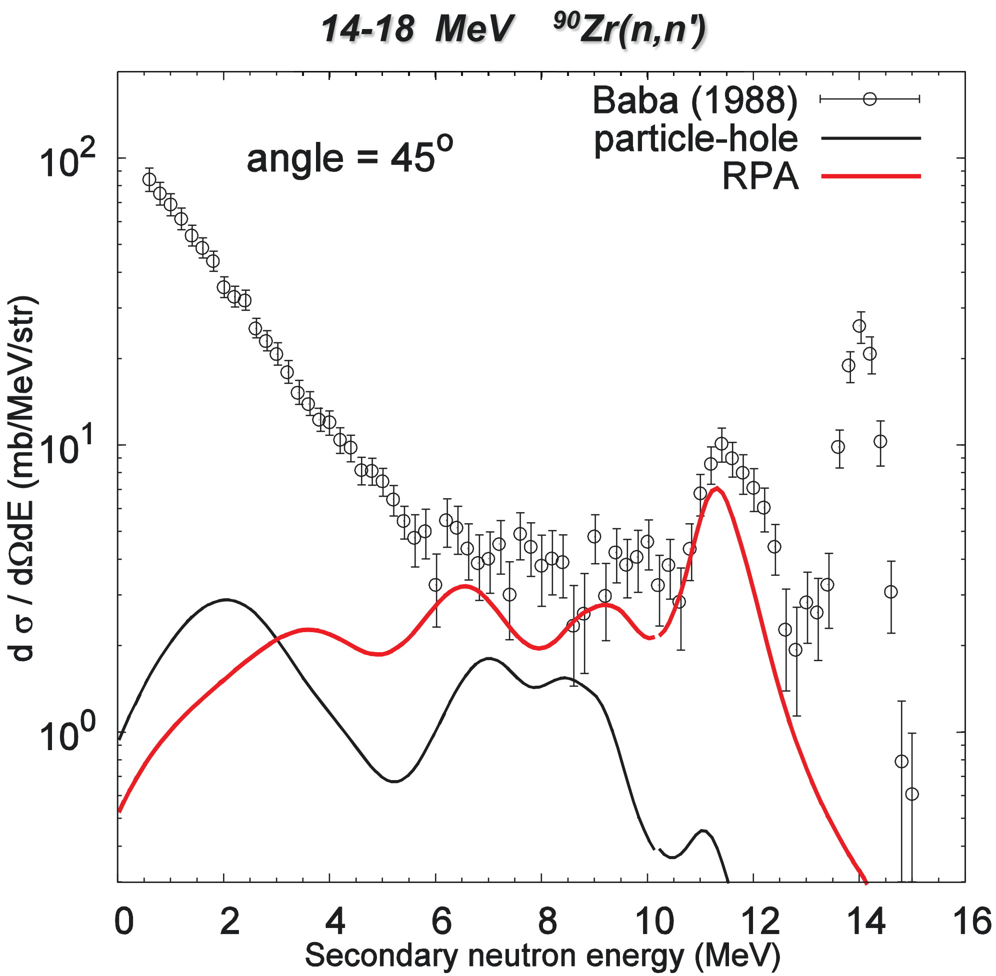
**Deformed nuclei**

⇒ **Microscopic structure from QRPA (complex & time consuming)**

# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (2/5)

## Microscopic description of target structure:

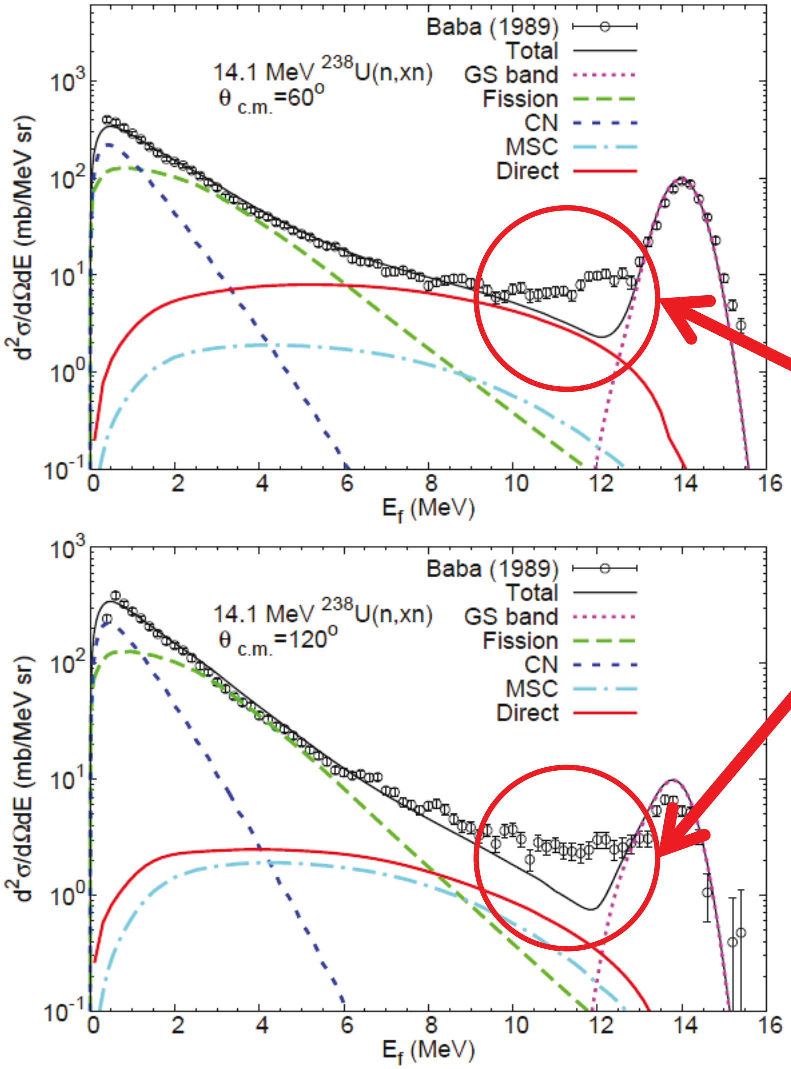
- **RPA**/D1S (collective levels)
- **particle-hole** (no collectivity).




⇒ **Microscopic structure = collective levels essential**

# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (3/5)

## Phenomenological model

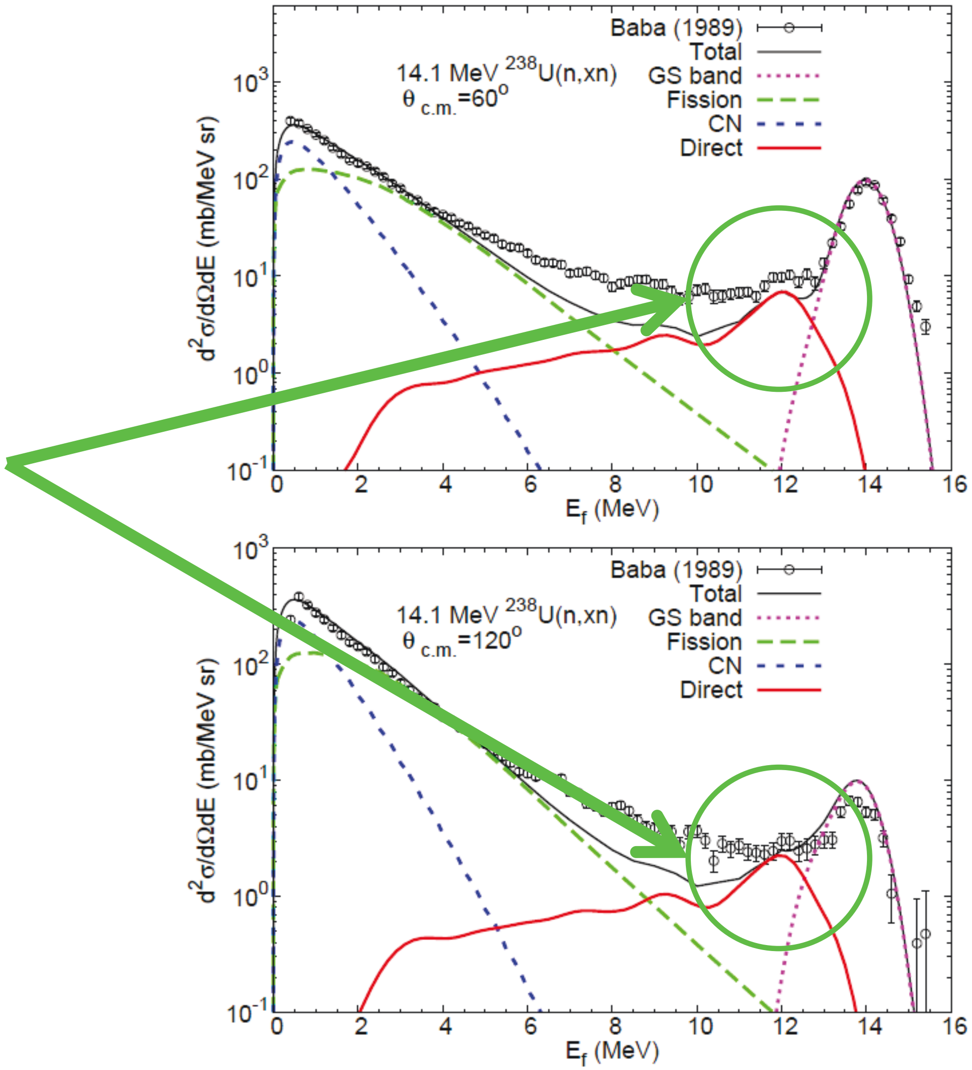



**Something missing here**
**Problem solved by adding ad-hoc Collective states in ENDF files**

# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (3/5)

## Microscopic model

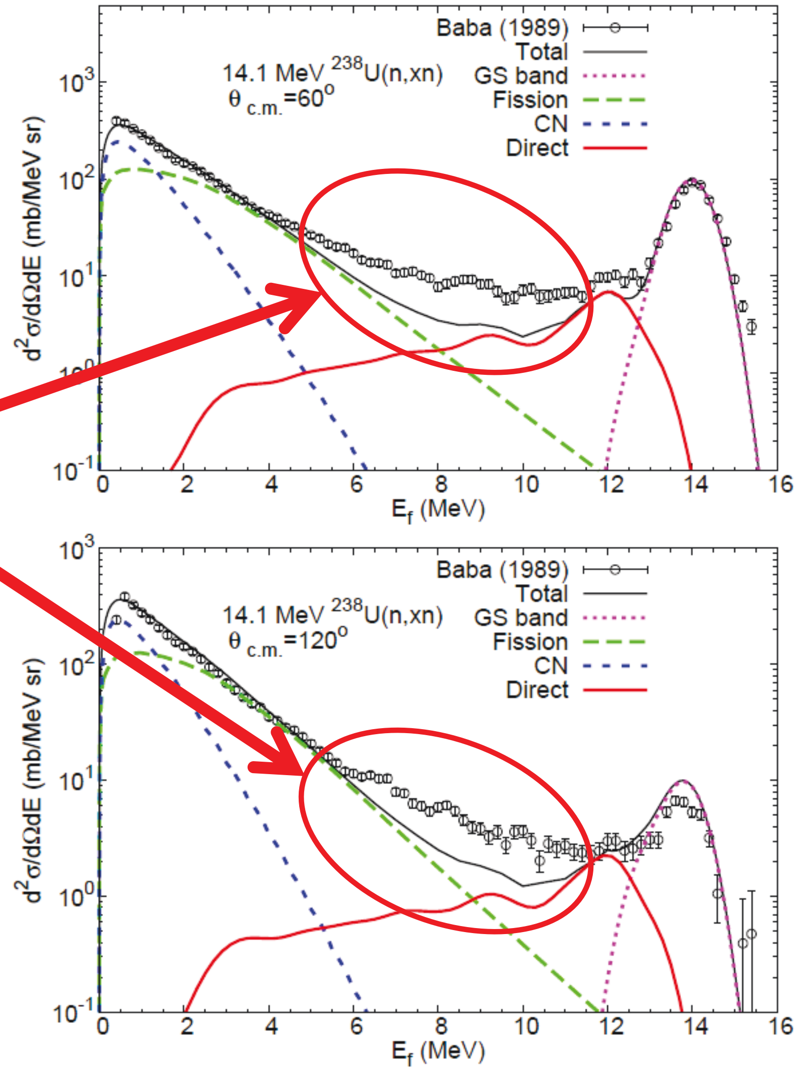
**Problem solved accounting Correctly for collective levels (no ad-hoc)**



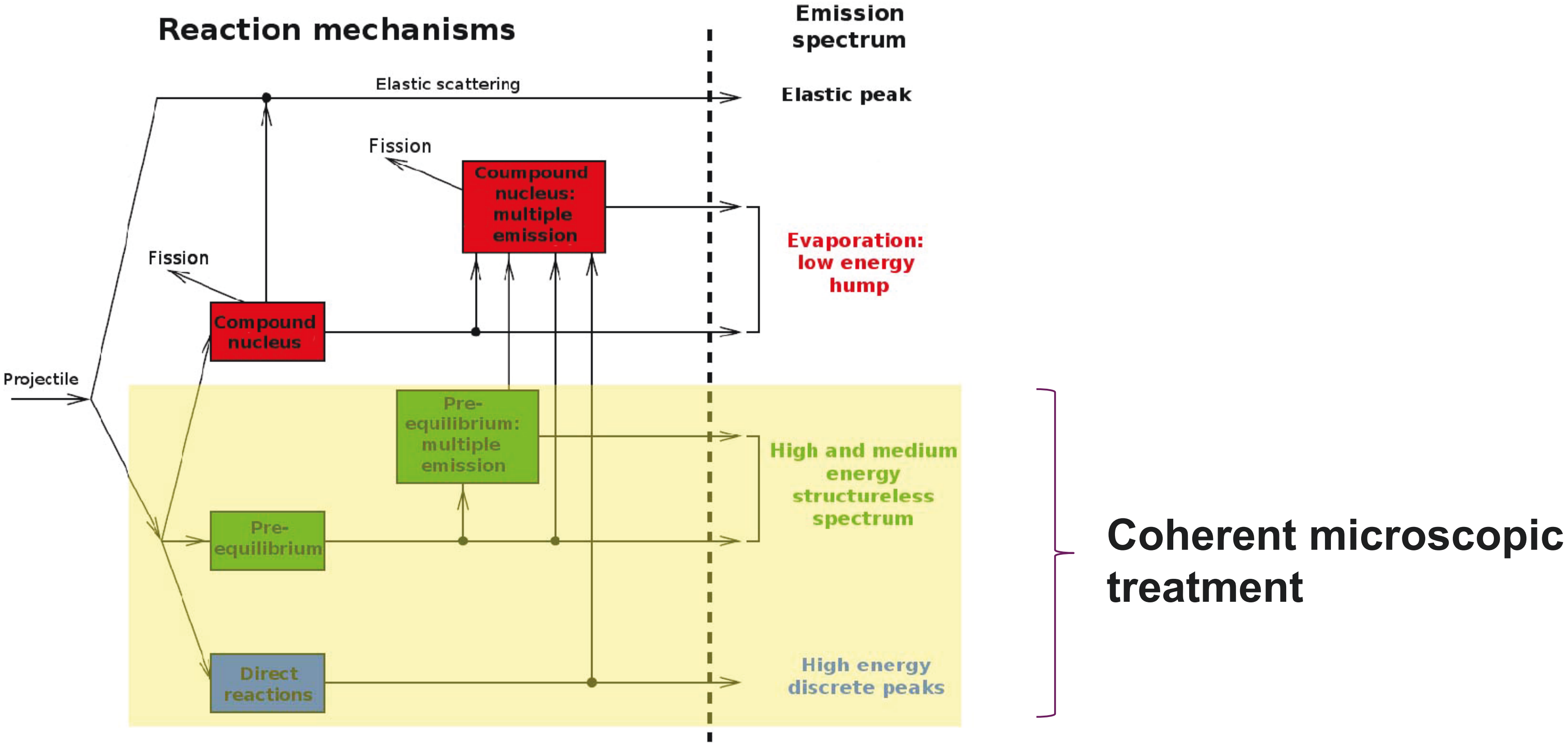
# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (3/5)

## Microscopic model

**Problem here probably due to 2nd step pre-equilibrium**

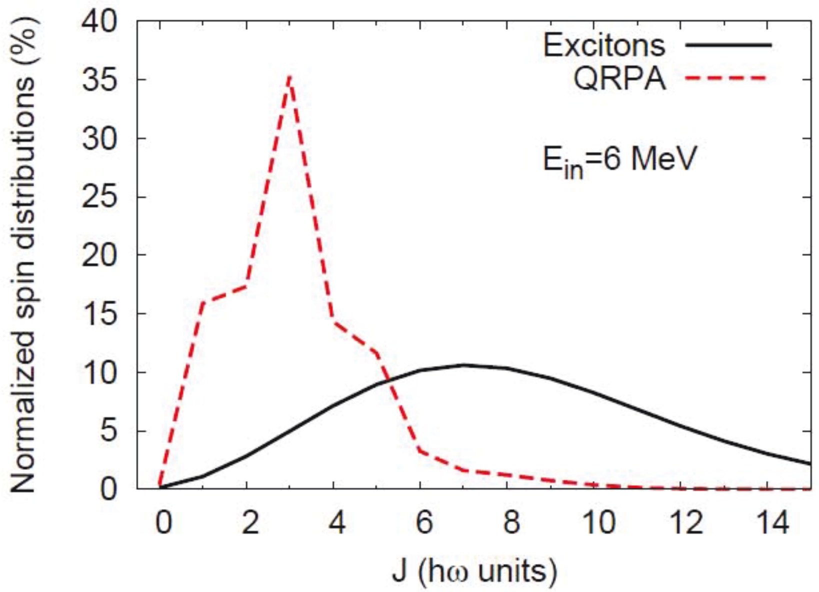


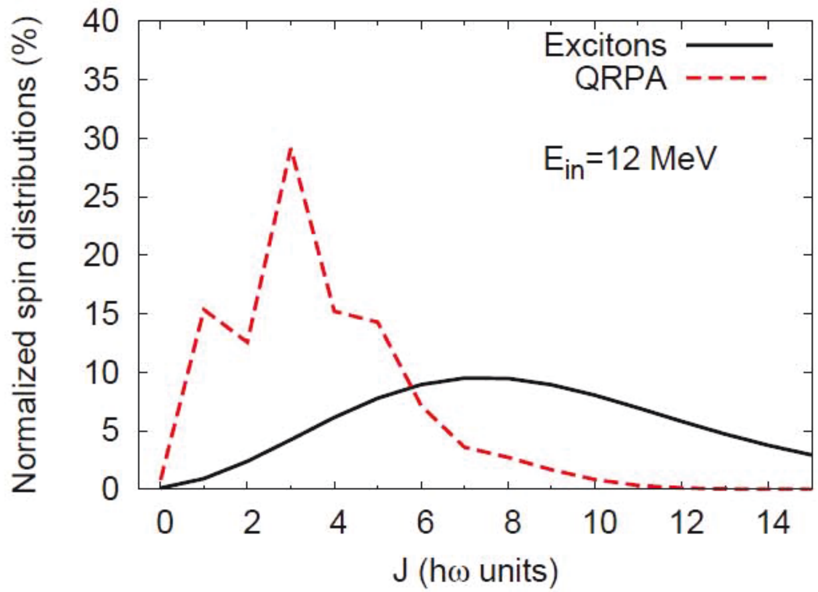
# FINE TUNING AND ACCURACY
## Microscopic pre-equilibrium modeling of cross sections (4/5)




⇒ **Modification of the compound nucleus spin population**

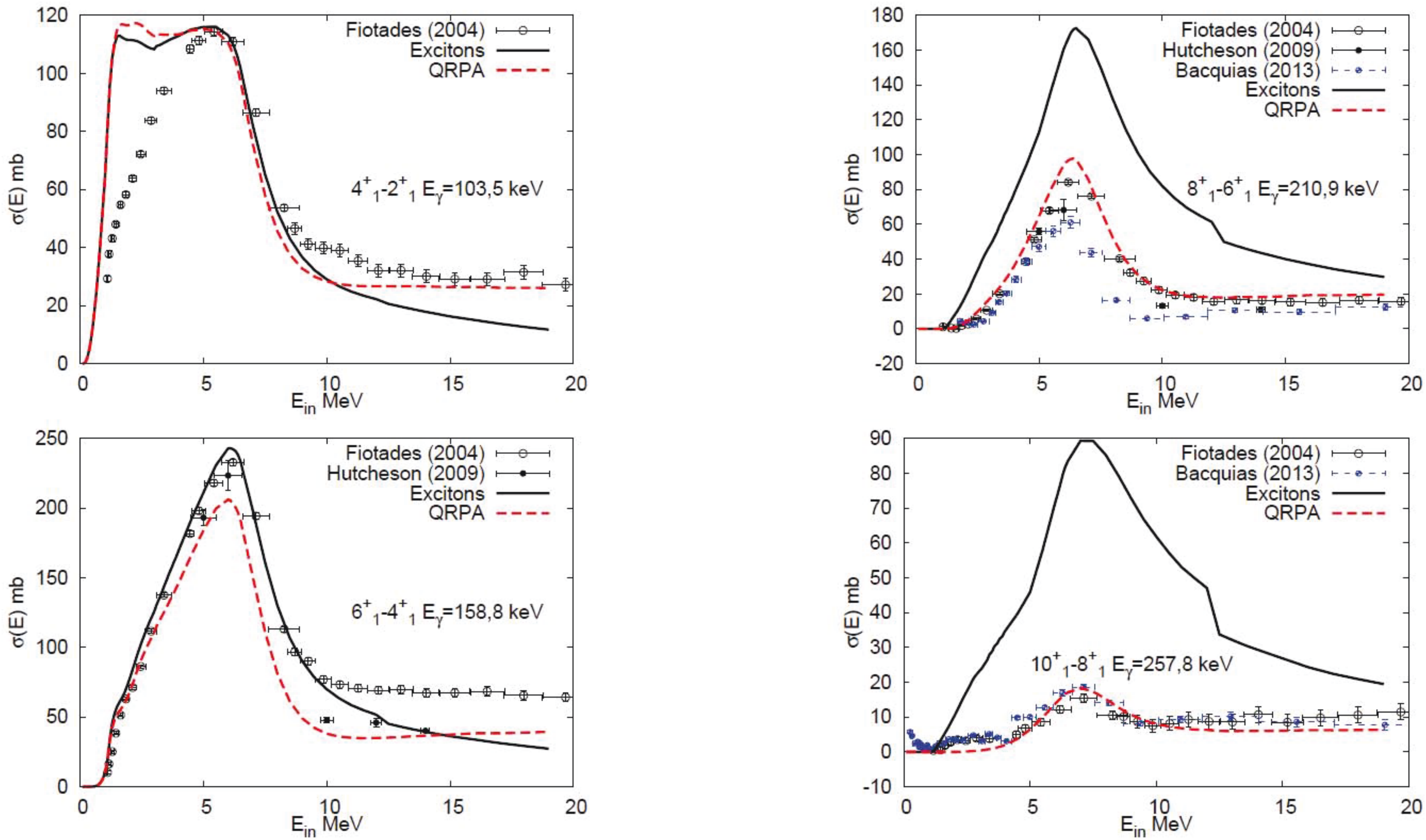
# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (4/5)

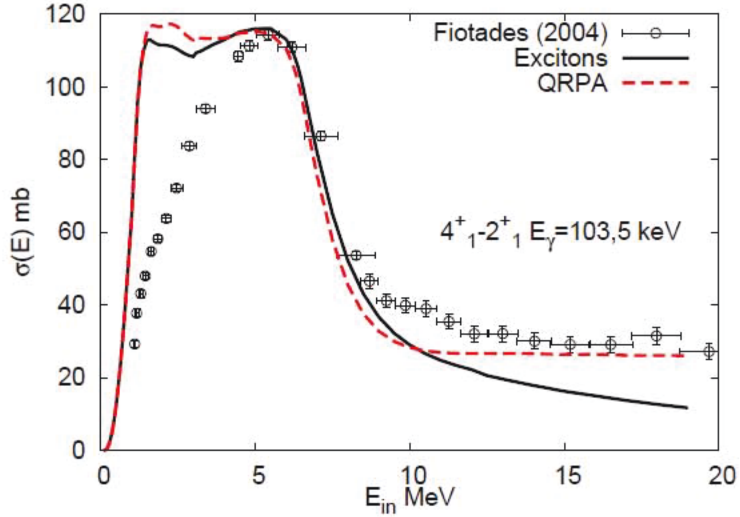



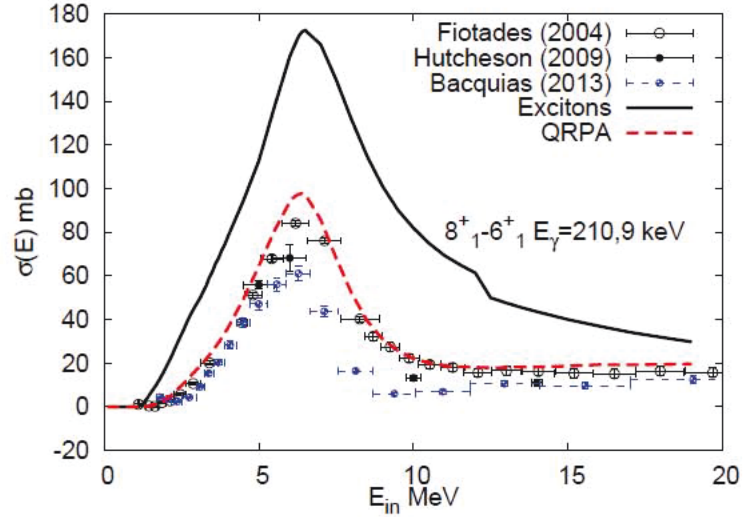

**⇒ Modification of the compound nucleus spin population**

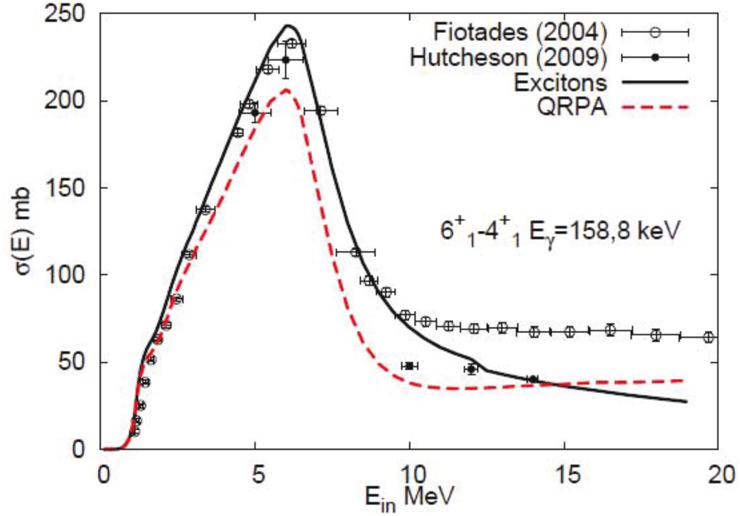
# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (5/5)

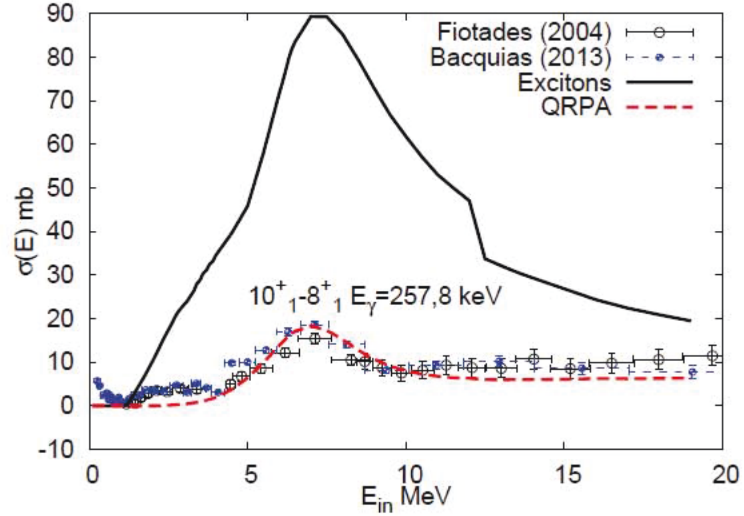


# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (5/5)

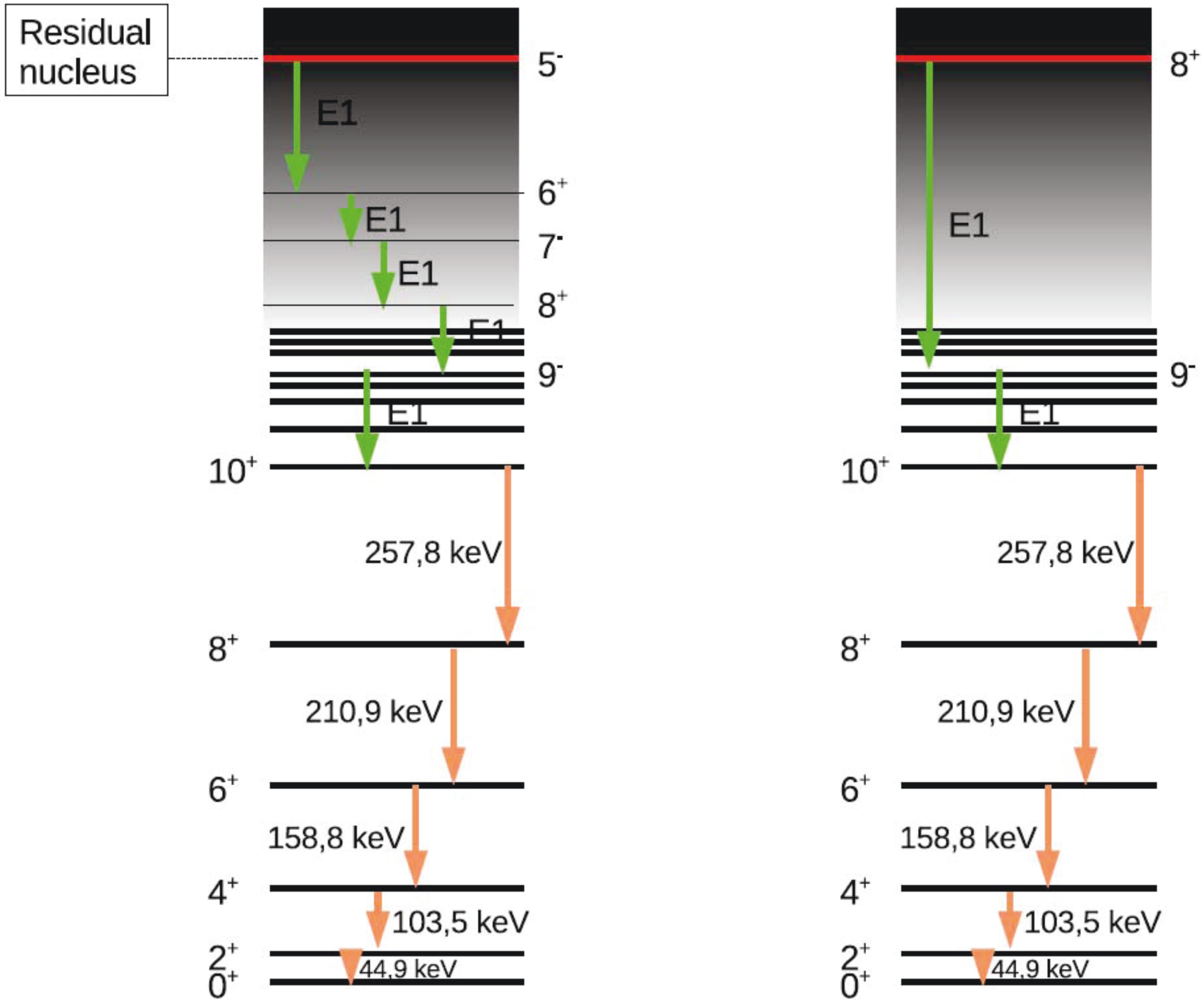


# FINE TUNING AND ACCURACY
# Microscopic pre-equilibrium modeling of cross sections (5/5)



# Content

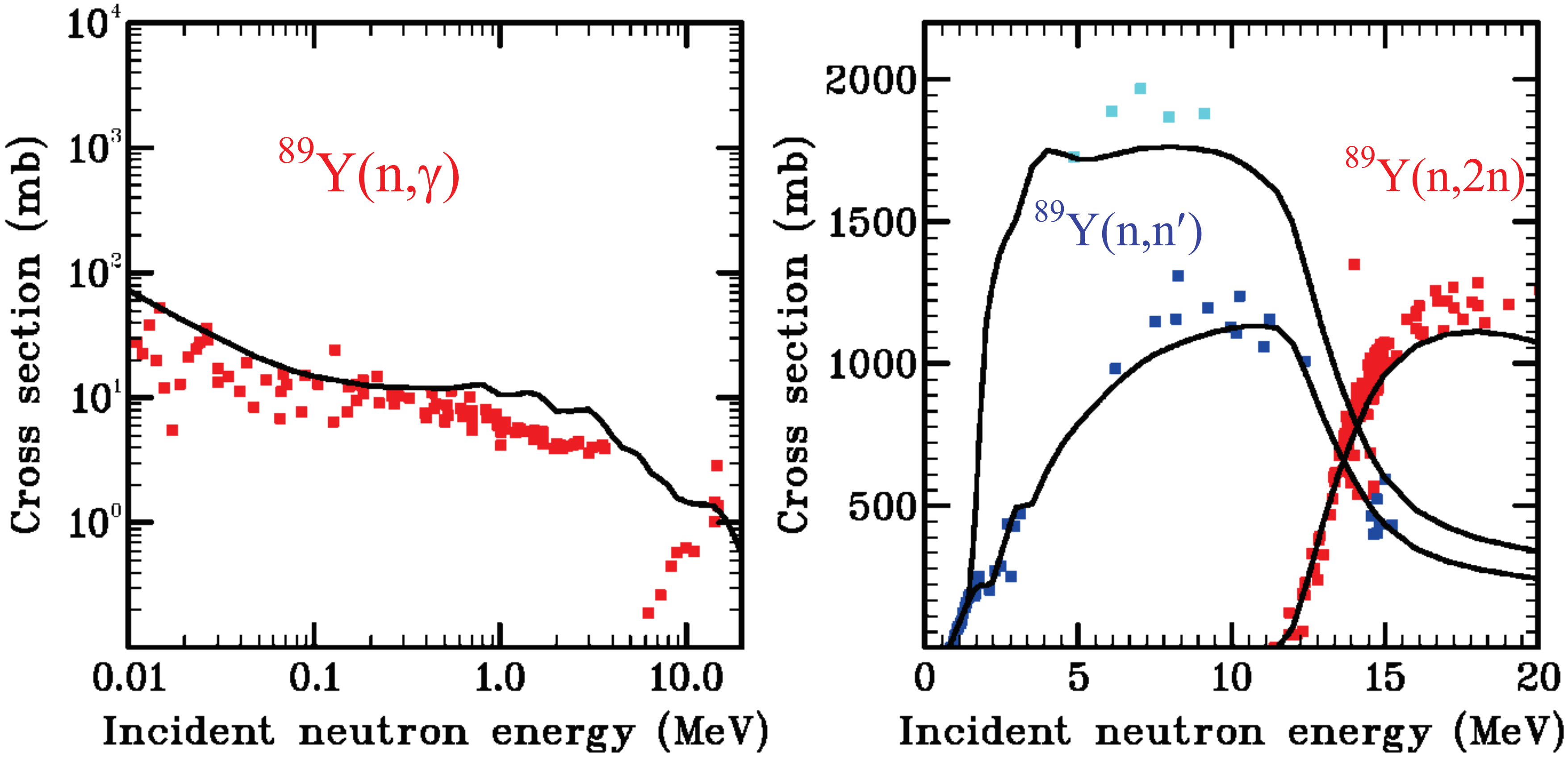
- Introduction
- General features about nuclear reactions
    - Time scales and associated models
    - Types of data needed
    - Data format = f (users)
- Nuclear Models
    - Basic structure properties
    - Optical model
    - Pre-equilibrium model
    - Compound Nucleus model
    - Miscellaneous : level densities, fission, capture
- **From in depth analysis to large scale production with TALYS**
    - General features about TALYS
    - Fine tuning and accuracy
    - **Global systematic approaches**
- **What remains to be done ?**

# GLOBAL SYSTEMATIC APPROACHES

- **Adjusting Nuclear level densities**
- **Astrophysical r-process**
- **Global trends in cross sections : isolating/solving problems**
- **Total Monte Carlo and covariances**
- **TENDL**

# GLOBAL SYSTEMATIC APPROACHES
## Adjusting level densities (1/4)

$$\rho_{renorm}(U) = e^{\alpha \sqrt{(U - \delta)}} \rho_{global}(U - \delta)$$



# GLOBAL SYSTEMATIC APPROACHES
## Adjusting level densities (1/4)

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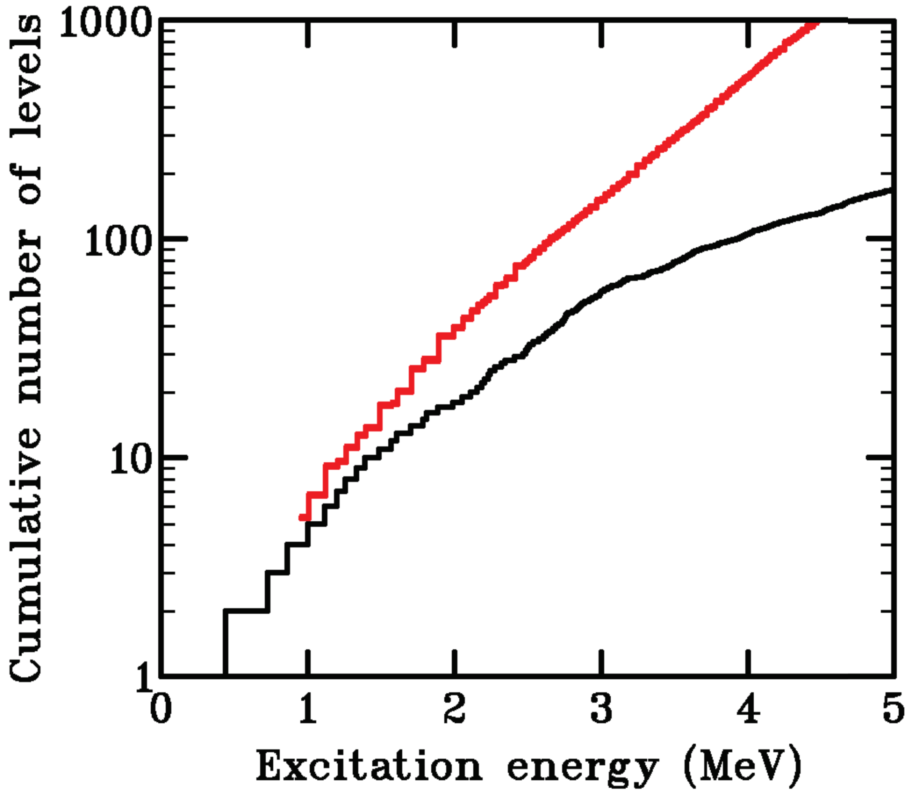


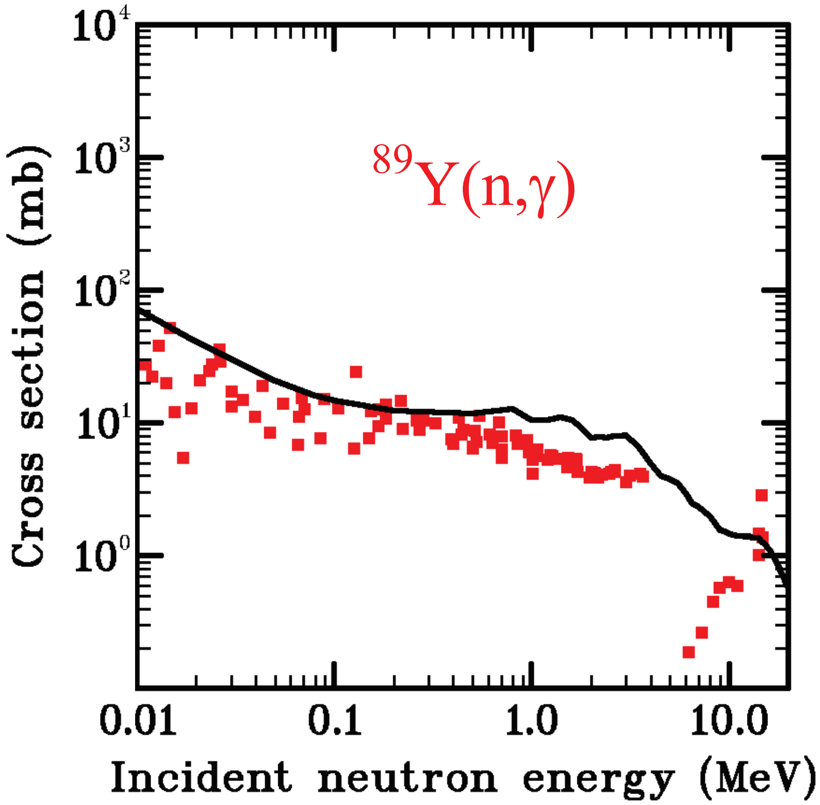

# GLOBAL SYSTEMATIC APPROACHES
## Adjusting level densities (1/4)

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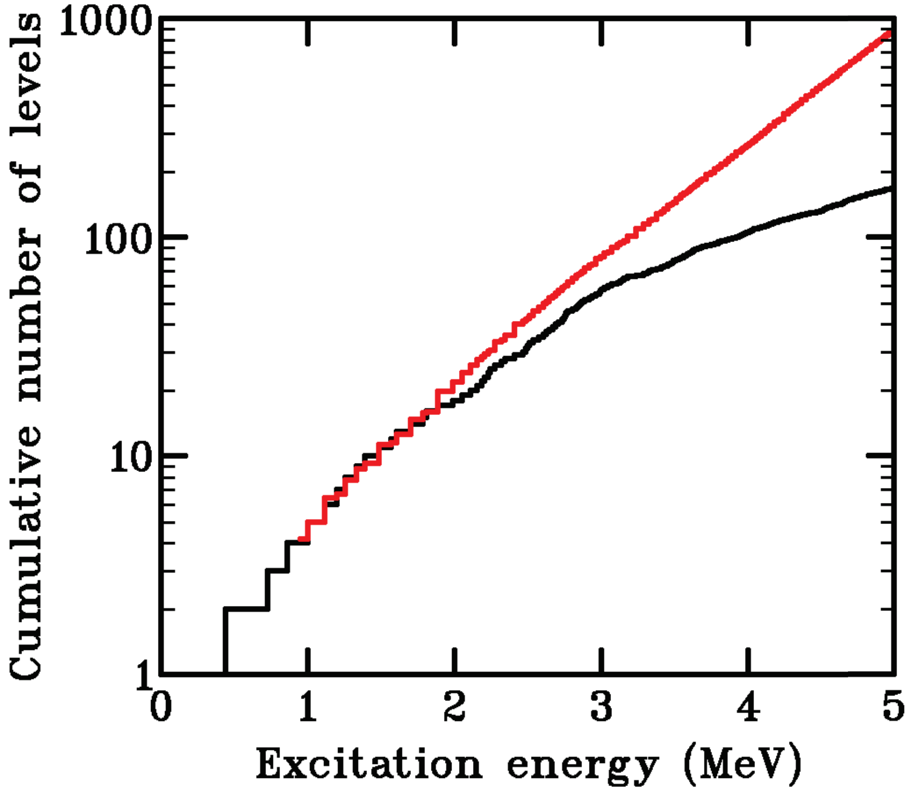
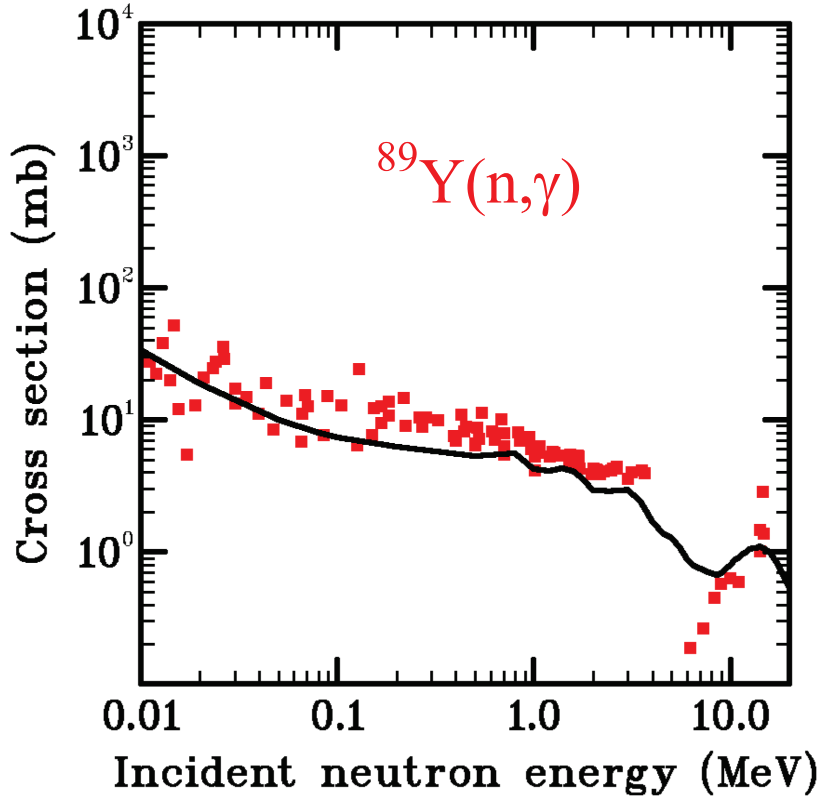


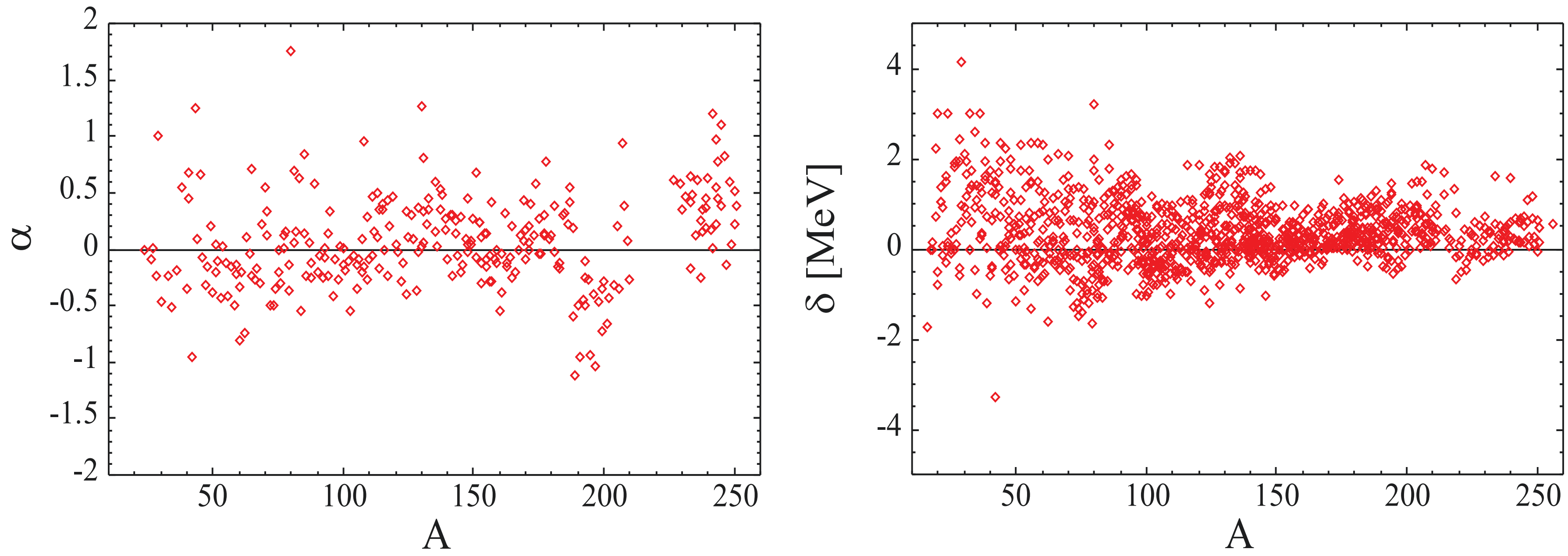



# GLOBAL SYSTEMATIC APPROACHES
## Adjusting level densities (2/4)



*See NPA 810 (2008) 13 for details*

α and δ adjusted to fit discrete levels (≈ 1200 nuclei) and $D_0$'s (≈ 300 nuclei) using the TALYS code



# GLOBAL SYSTEMATIC APPROACHES
## Adjusting level densities (3/4)

**Levels density models implemented/adjusted in TALYS**

- **Gilbert-Cameron model + Ignatyuk**

  ⇒ **Default**

- **Back-Shifted Fermi Gas model + Ignatyuk**

  ⇒ **Less accurate than GC at low energy**

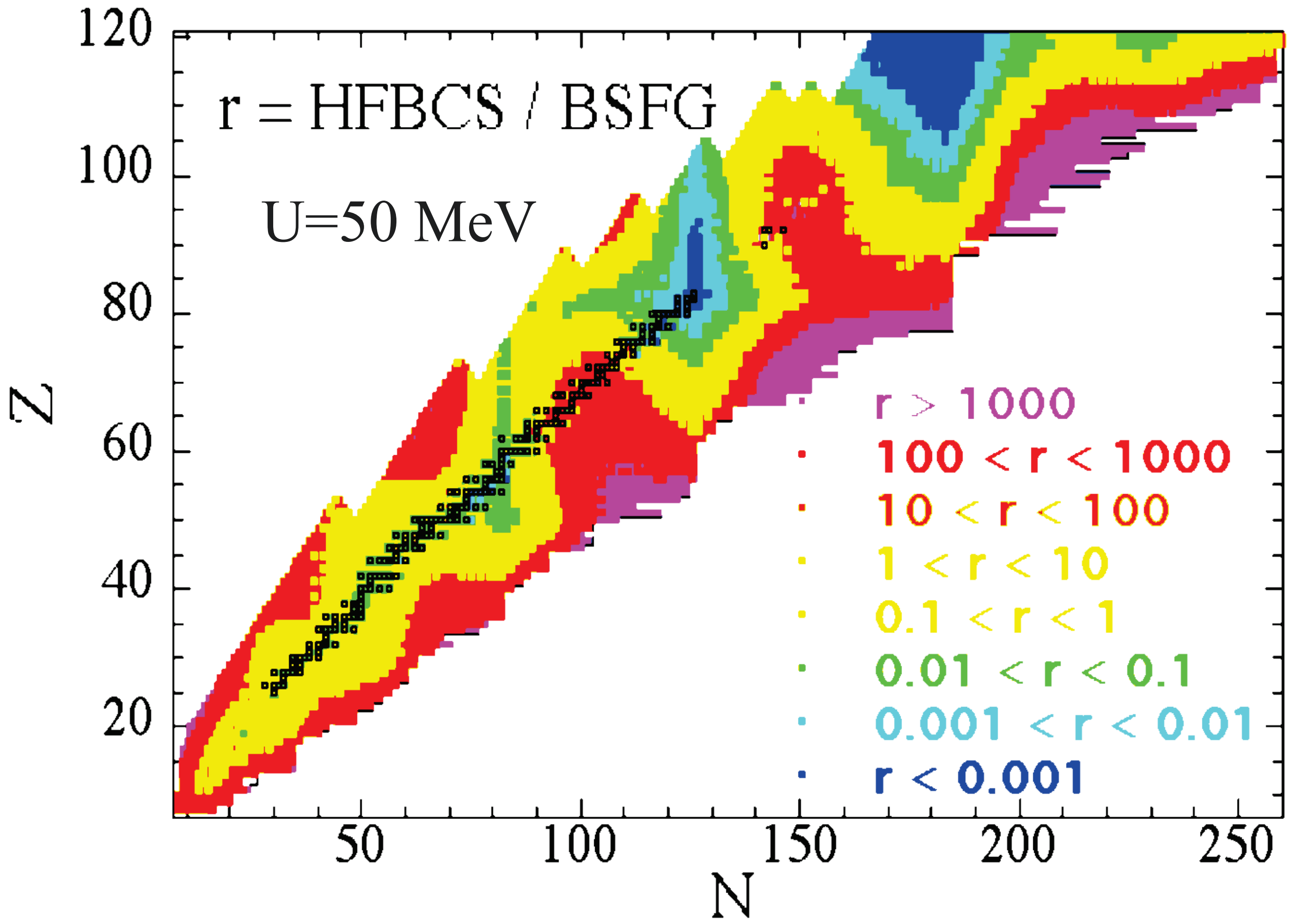
- **(Generalized) Superfluid model**

  ⇒ **More rigourous treatment of pairing correlation at low energy**
  ⇒ **Fermi gas + Ignatyuk law above some critical energy**
  ⇒ **(Explicit treatment of collective effects)**

- **Combinatorial approach**

  ⇒ **Using Skyrme or Gogny single particle levels**
  ⇒ **Using Gogny temperature dependent treatment**

# Microscopic NLD formula based on HF-BCS
# vs
# Analytical shell-corrected Back-Shifted Fermi Gas



# Solar abundancies for 140 < A < 200 : r-nuclei ?

## Two options :

- Supernovae :
  - Matter ejection without any problem +++
  - Great sensitivity to thermodynamical conditions - - -
  - No clearly identified astrophysical site - - -
  - Failure of explosion models - - -

- Neutron stars collisions :
  - Enough neutrons +++
  - Binary systems abundancies ? - - -
  - Matter ejection ? - - -
  - Grosse sensibilité aux modèles de fission - - -

# GLOBAL SYSTEMATIC APPROACHES
## Astrophysical r-process (1/4)

**Solar abundancies for 140 < A < 200 : r-nuclei ?**

**Two options :**

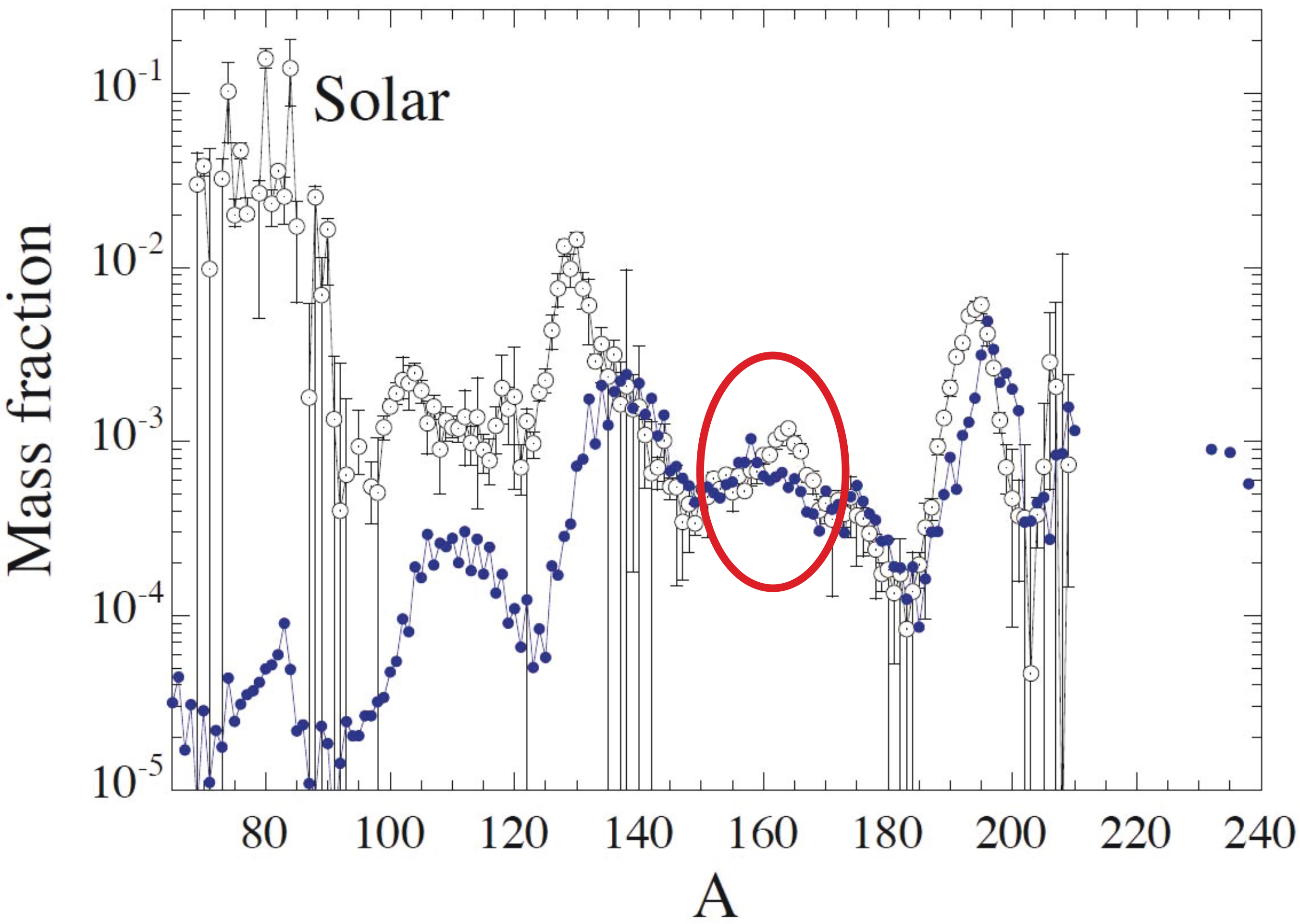
- **Supernovae :**

| | |
|---|---|
| Matter ejection without any problem | +++ |
| Great sensitivity to thermodynamical conditions | - - - |
| No clearly identified astrophysical site | - - - |
| Failure of explosion models | - - - |

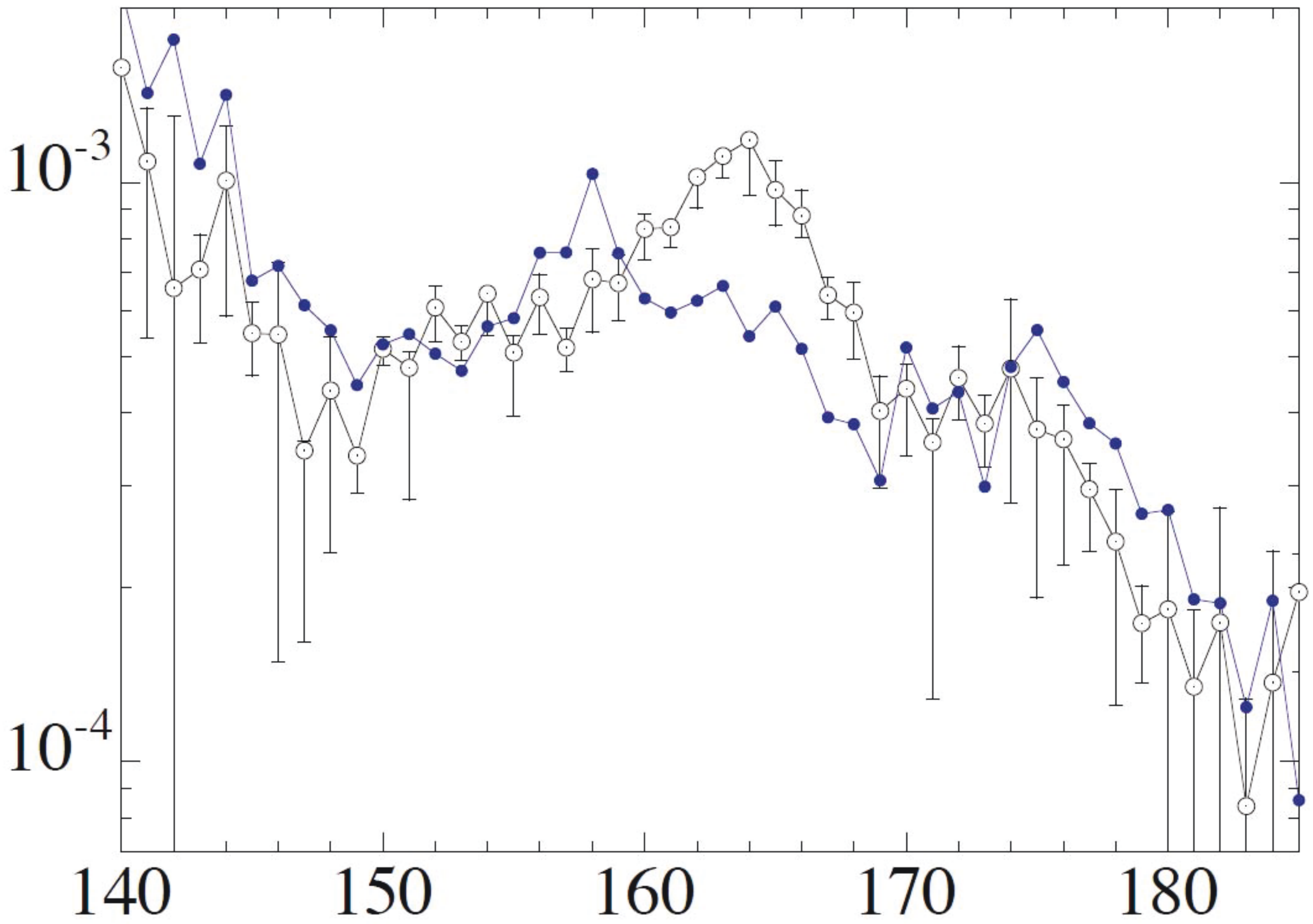
- **Neutron stars collisions :**

| | | |
|---|---|---|
| Enough neutrons | | +++ |
| Binary systems abundancies ? | Recently solved | +++ |
| Matter ejection ? | Recently solved | +++ |
| Grosse sensibilité aux modèles de fission | | - - - |

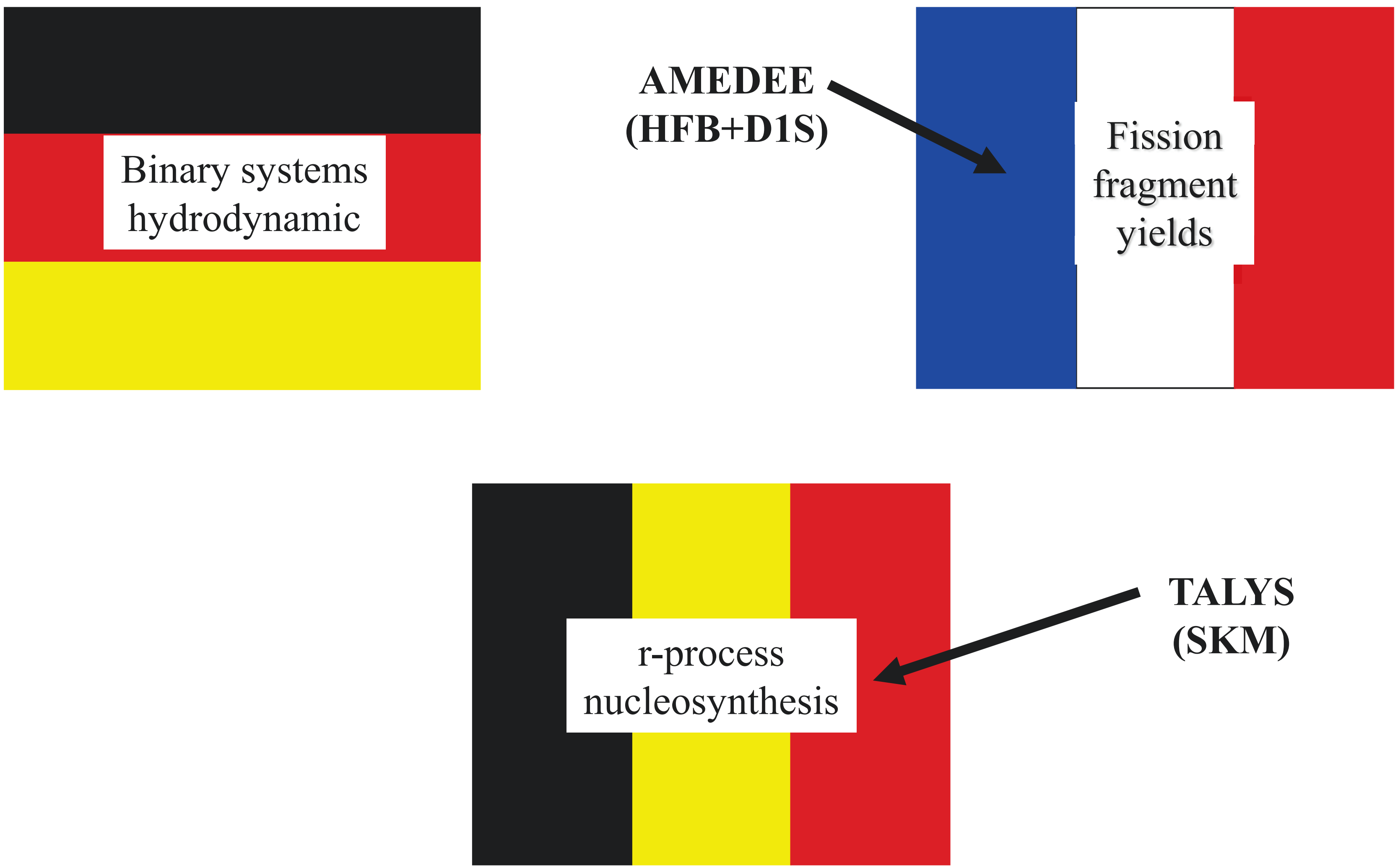
## Solar abundancies for 140 < A < 200 : situation before 2013 ?



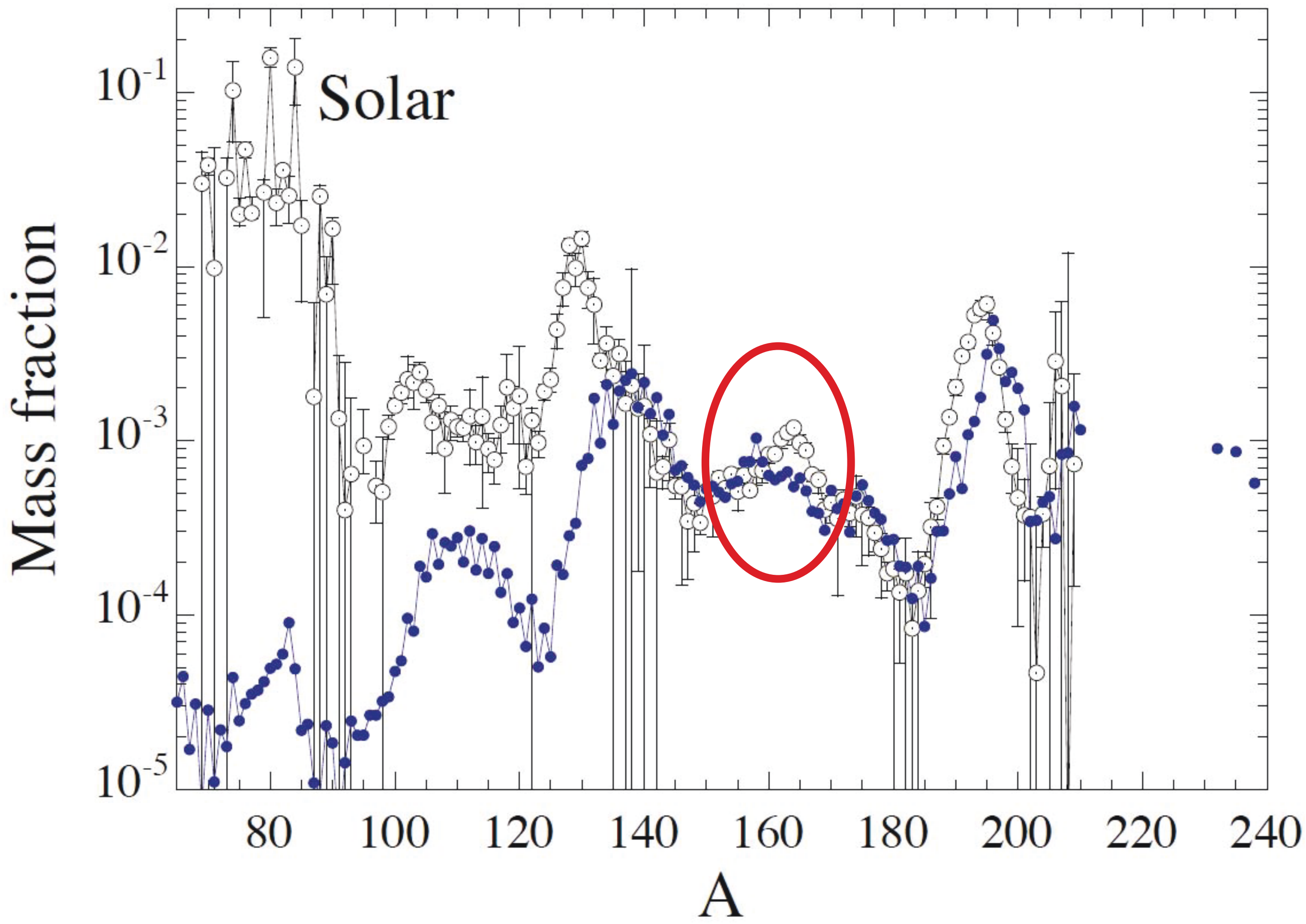
## Solar abundancies for 140 < A < 200 : situation before 2013 ?



# GLOBAL SYSTEMATIC APPROACHES
## Astrophysical r-process (3/4)

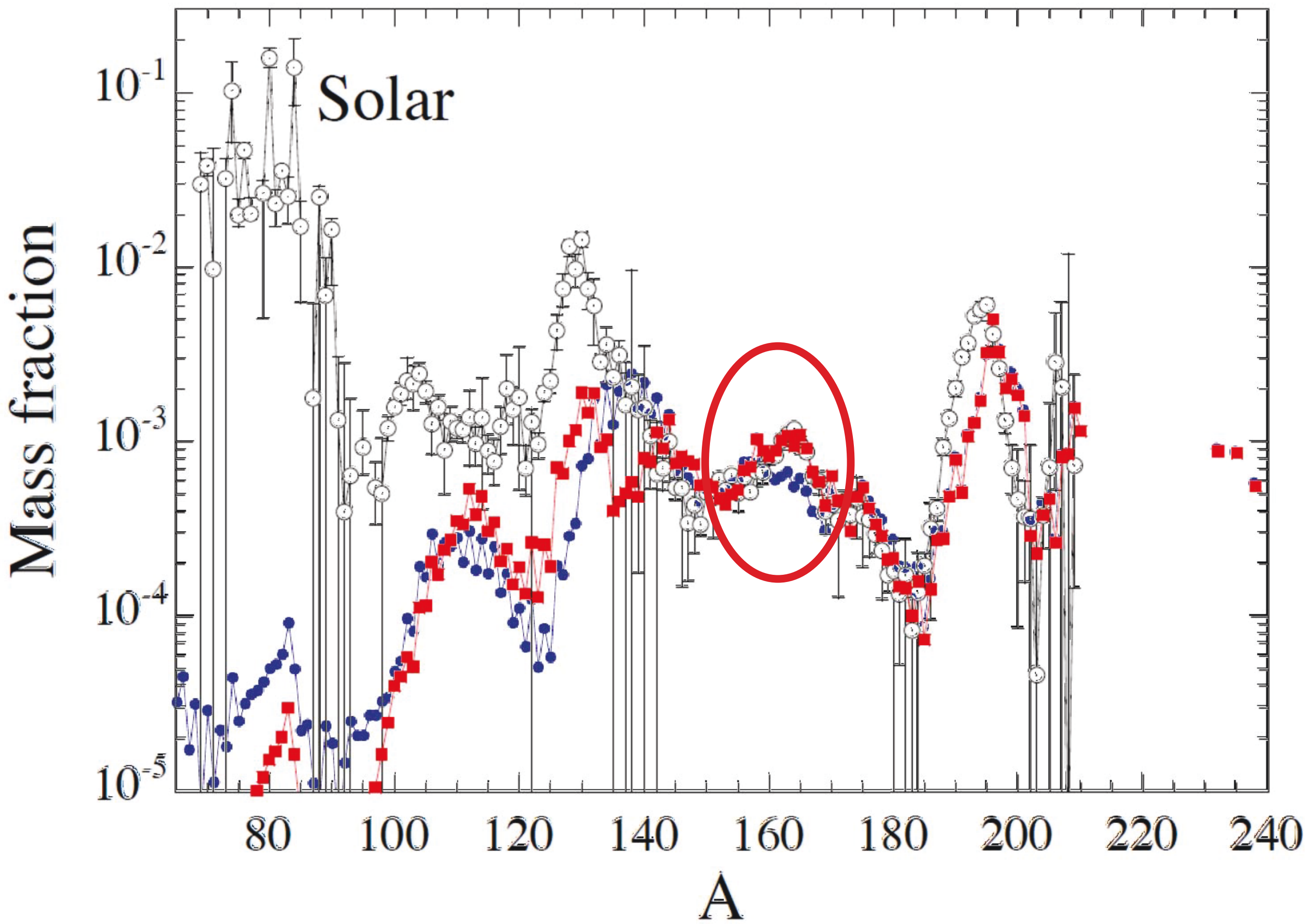


**Solar abundancies for 140 < A < 200 : situation before 2013 ?**

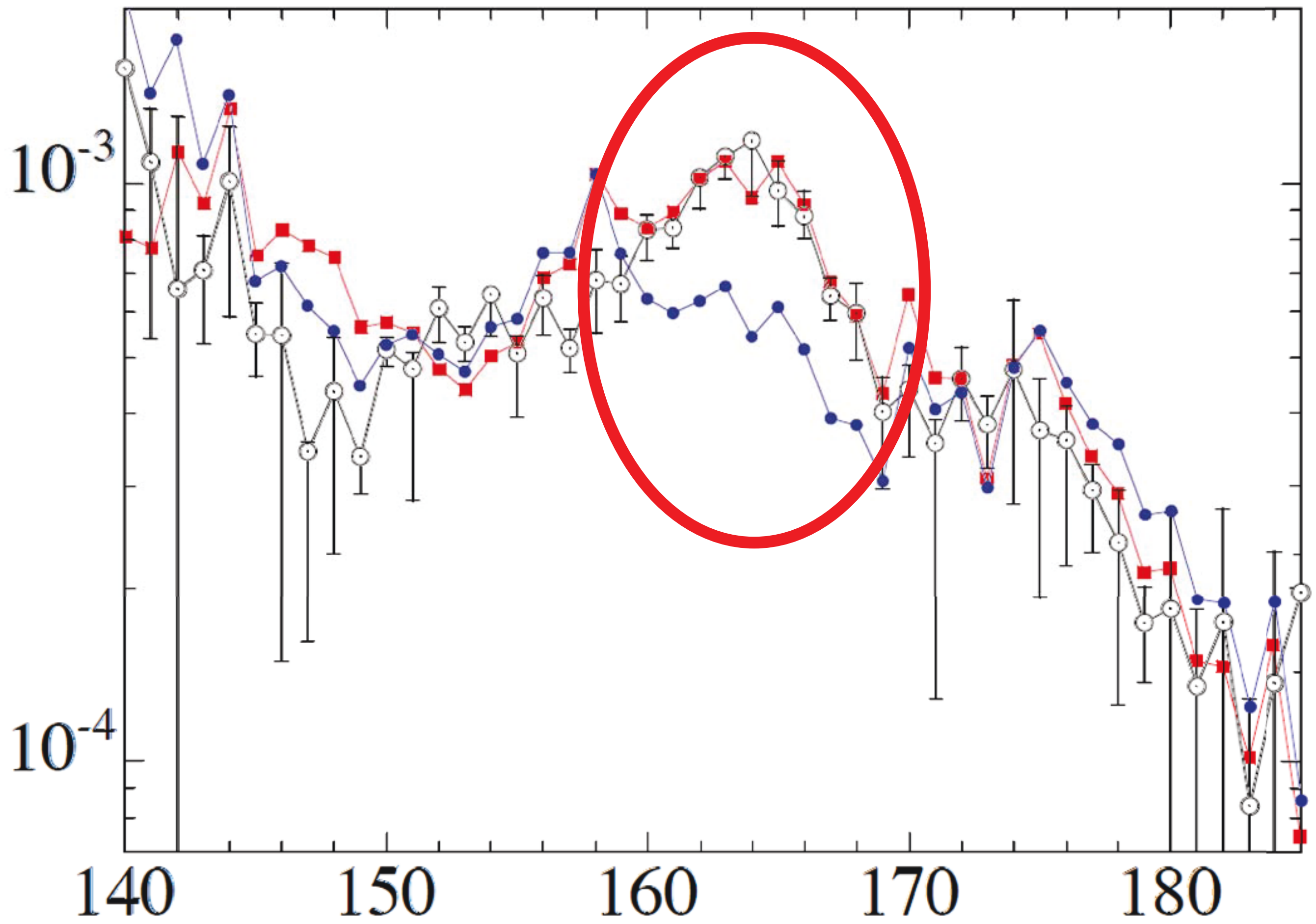


# GLOBAL SYSTEMATIC APPROACHES
## Astrophysical r-process (4/4)

**Solar abundancies for 140 < A < 200 : situation in 2013**



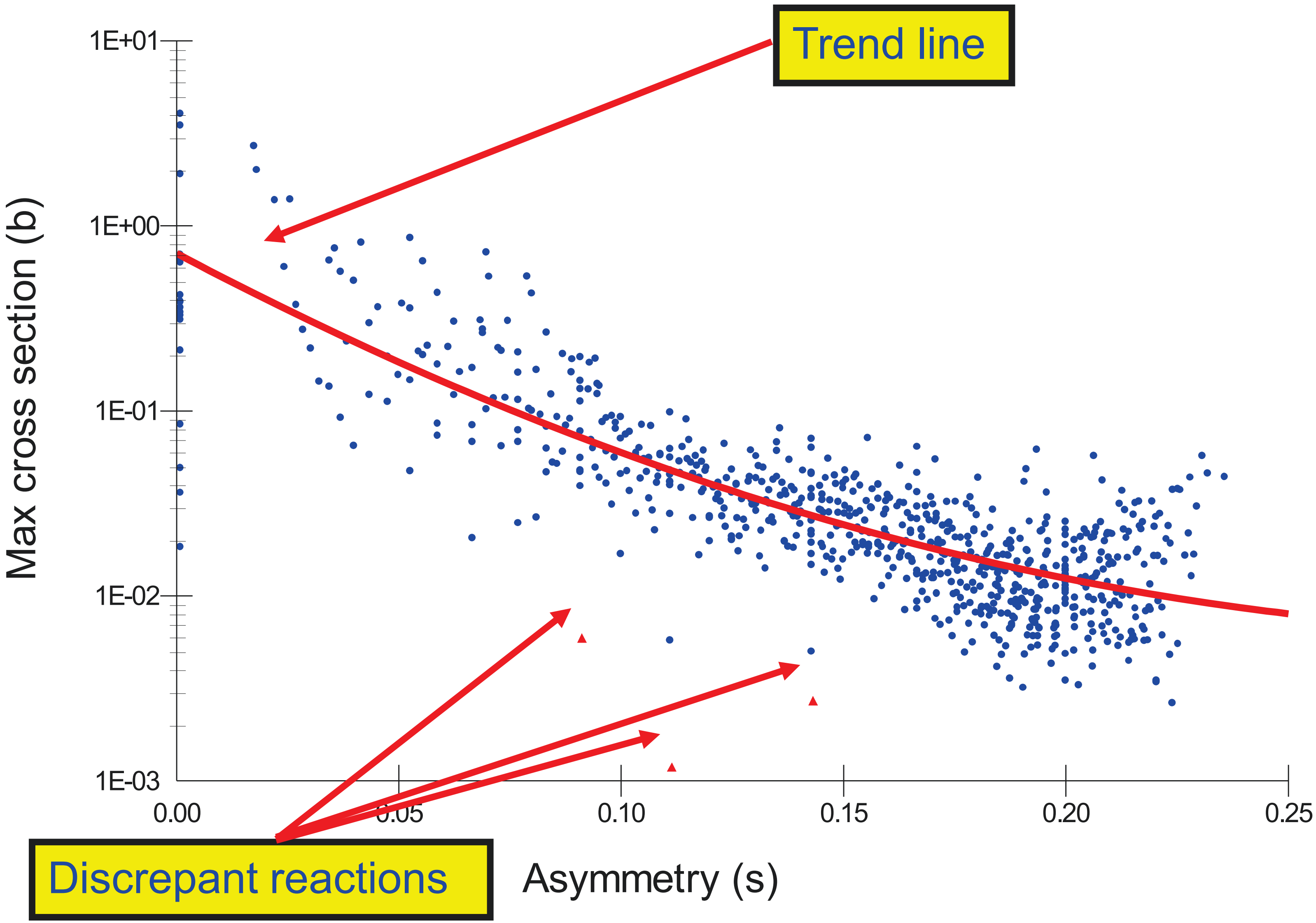
# GLOBAL SYSTEMATIC APPROACHES
## Astrophysical r-process (4/4)




More details for discussions/explanations in PRL 111, 242502 (2013)

# GLOBAL SYSTEMATIC APPROACHES
## Global trends in cross sections (1/2)

## Testing TALYS trends: (n,p) (J. Kopecky)



# Global comparison with experiment

**Can we compare all existing experimental data with nuclear models?**

Nuclear model codes are ready: TALYS + smart script: 1 day (20 MeV) – 1 week (200 MeV) calculation time

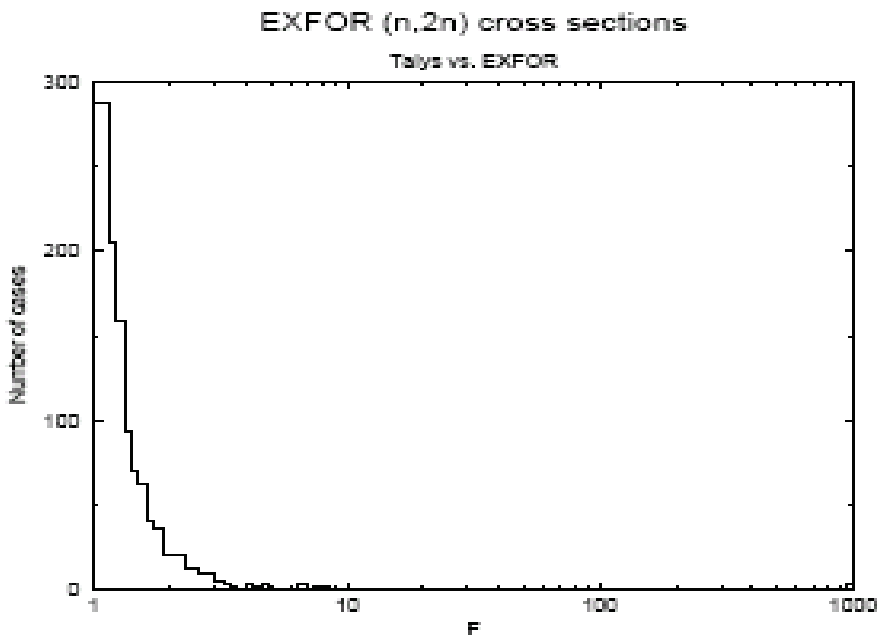
…but the experimental data collection (EXFOR) is not.

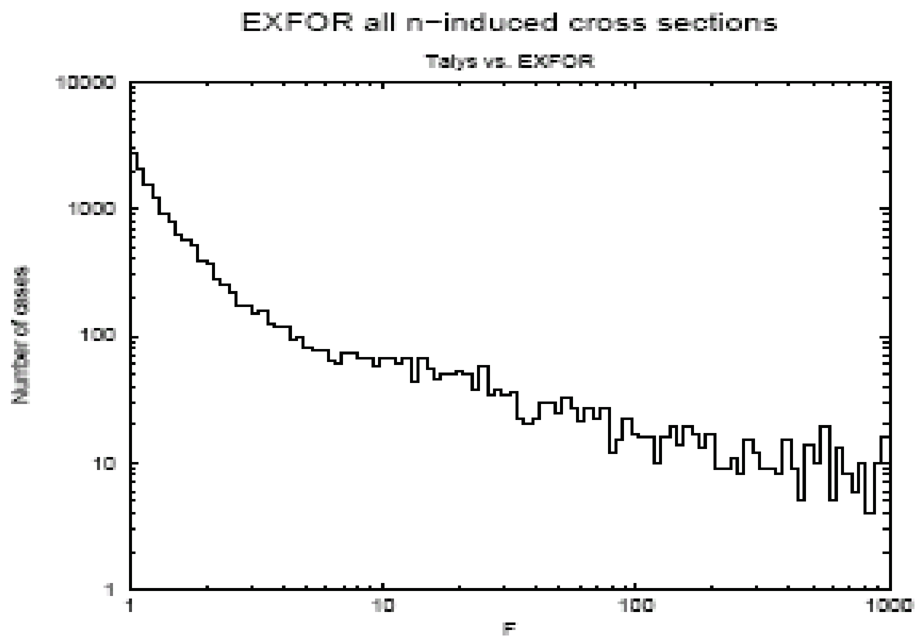
**A working group of the NEA has helped for this: Turn EXFOR into a database**

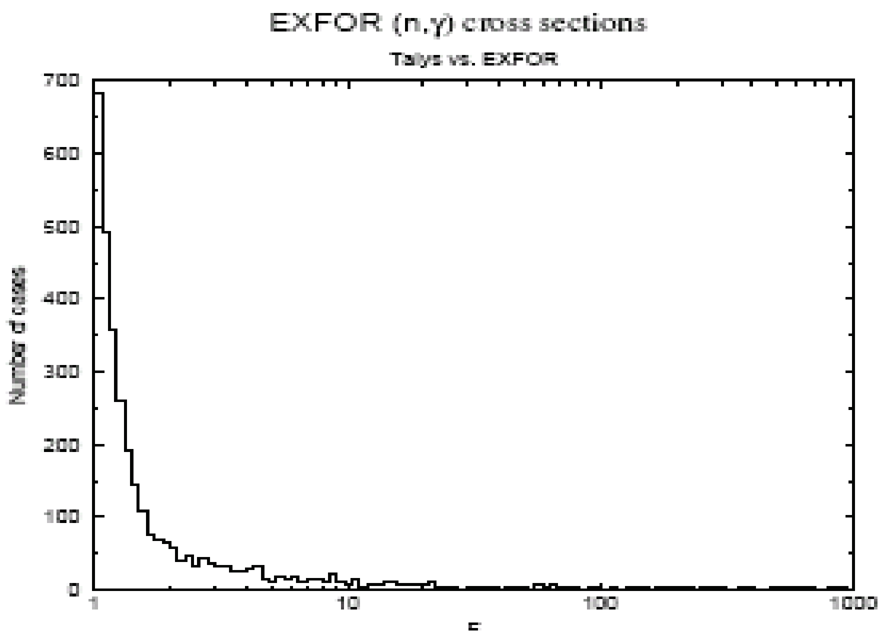
1. This will help to improve nuclear models + parameters
2. This will help to clean up (bugs) in EXFOR

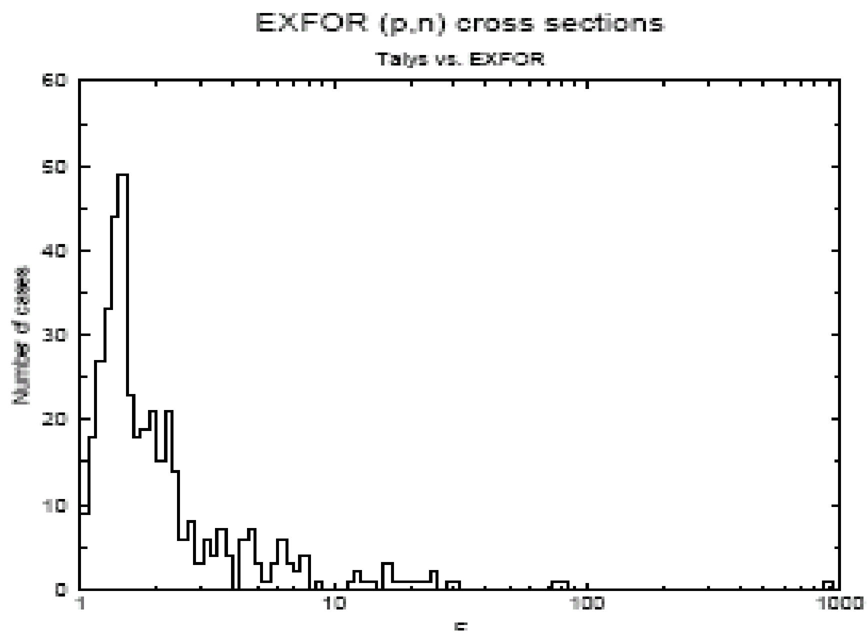
**Current situation: 16000 exp. data sets (400 000 points) can be automatically compared with TALYS**

# GLOBAL SYSTEMATIC APPROACHES

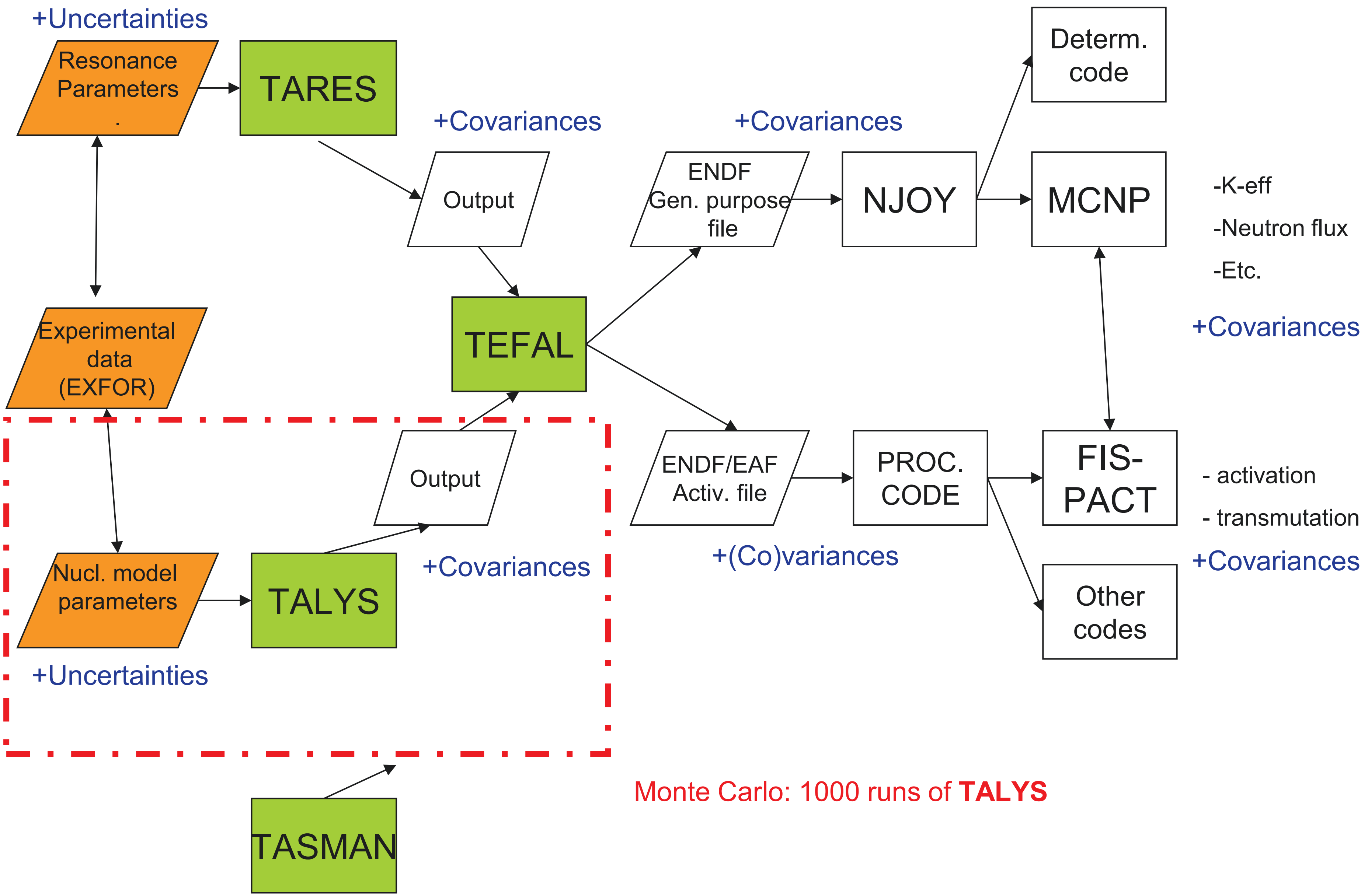


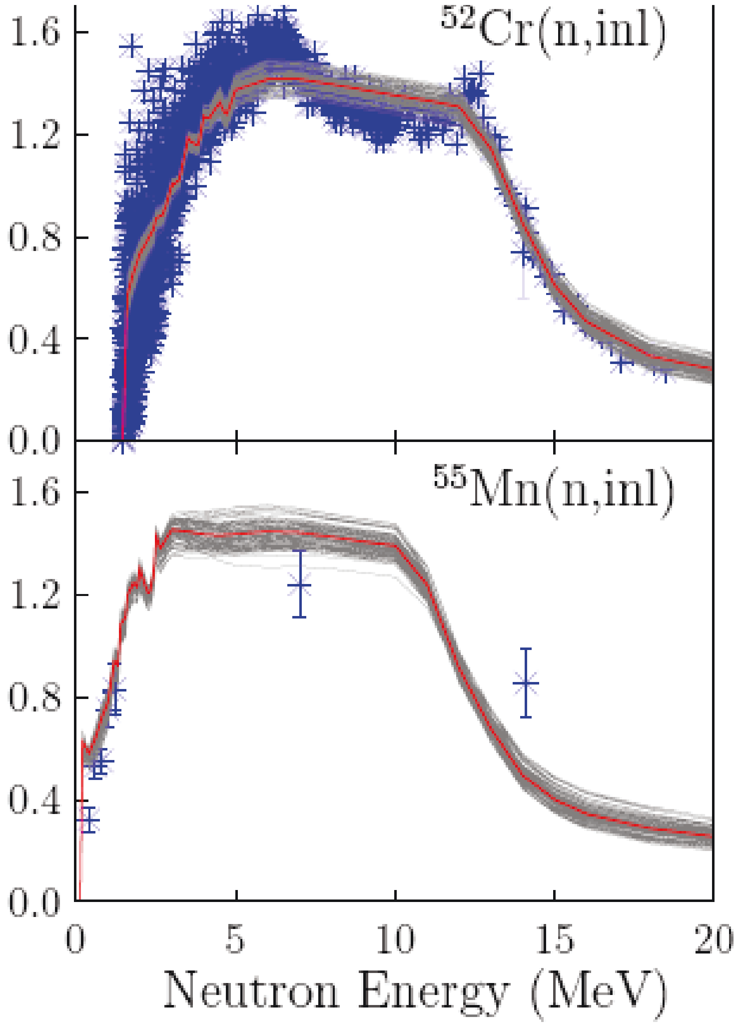



# GLOBAL SYSTEMATIC APPROACHES
## Covariances (1/2)



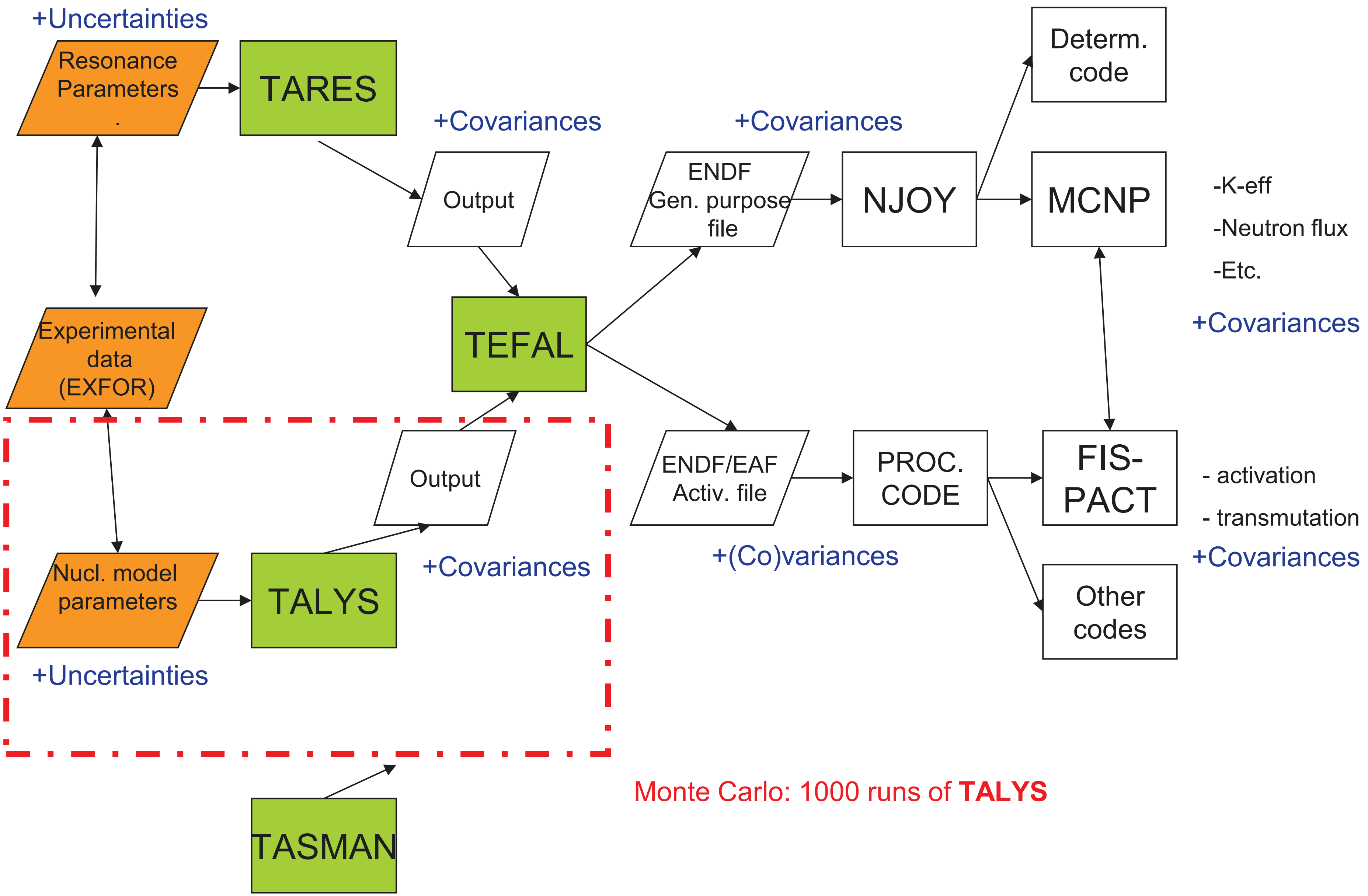

Monte Carlo: 1000 runs of **TALYS**

## UNCERTAINTIES FROM RANDOM TALYS PARAMETERS

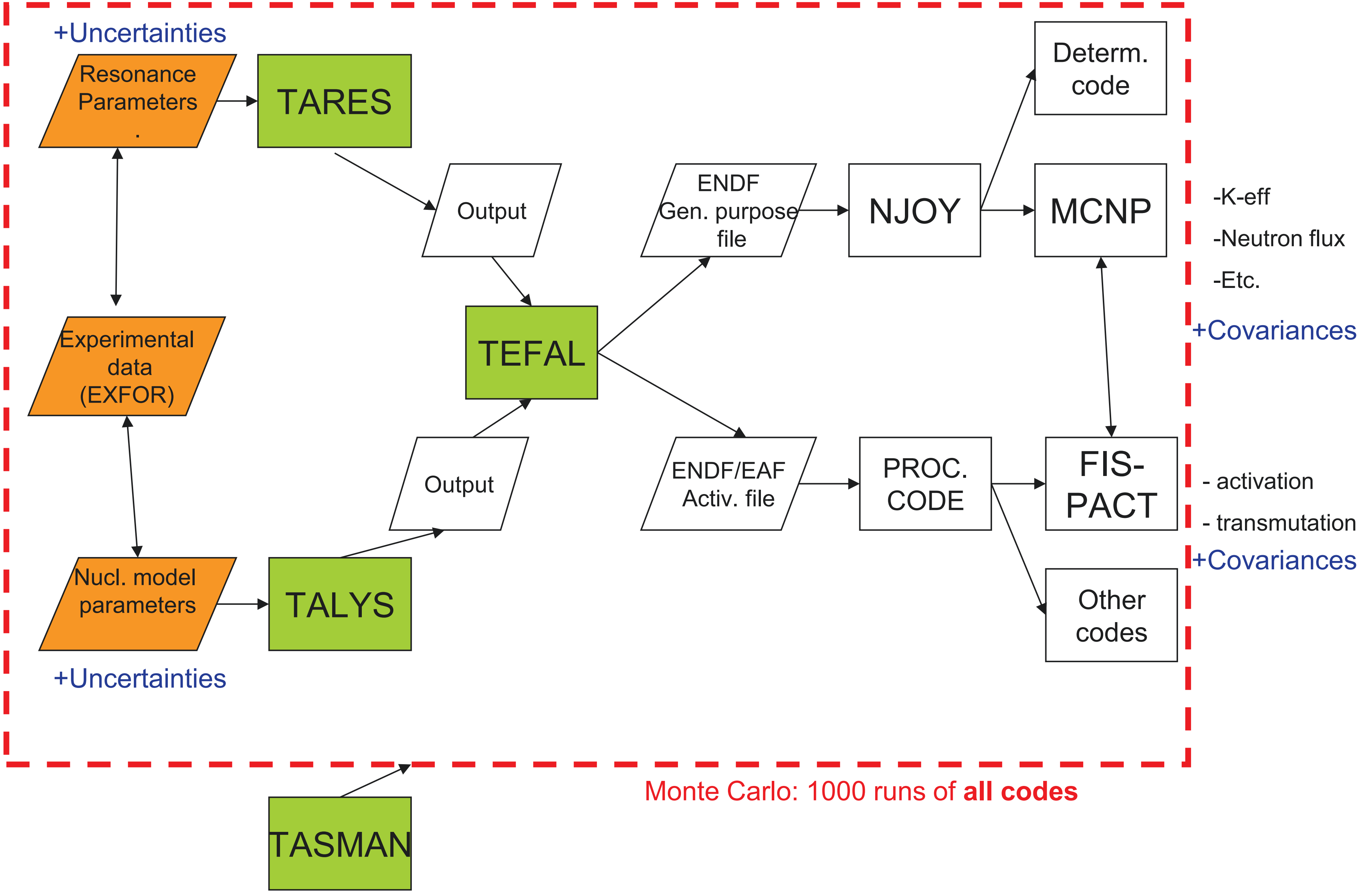



## + COVARIANCES FOR THE SAME PRICE

# GLOBAL SYSTEMATIC APPROACHES
## Covariances (1/2) : reminder



# GLOBAL SYSTEMATIC APPROACHES
# Total Monte Carlo (1/2)



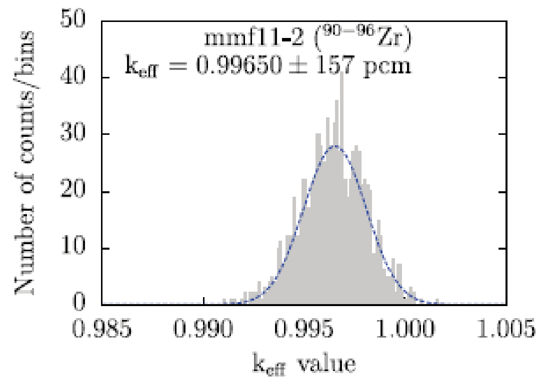
# TMC APPLICATION: CRITICALITY BENCHMARKS

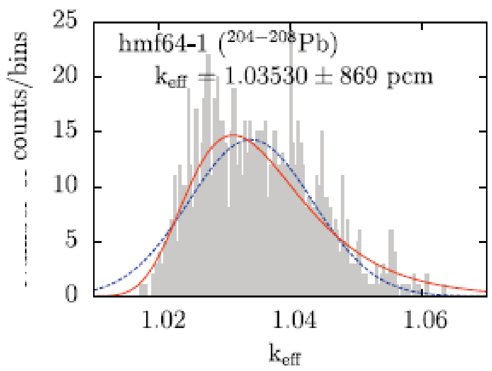
Total of 60000 random ENDF-6 files

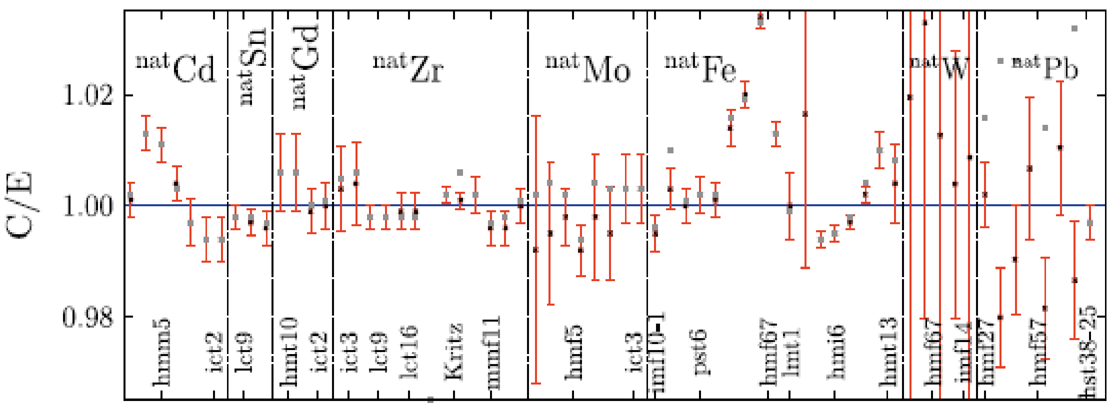
Sometimes deviation from Gaussian shape

*D. Rochman, A.J. Koning and S.C. van der Marck, ["Uncertainties for criticality-safety benchmarks and keff distributions"], Ann. Nuc. En. 36 810-831 (2009).*

**Yields uncertainties on benchmarks !**



# TENDL
# Talys Evaluated Nuclear Data Library (1/2)

## TALYS Evaluated Nuclear Data Library: TENDL-2008, …, TENDL-2014

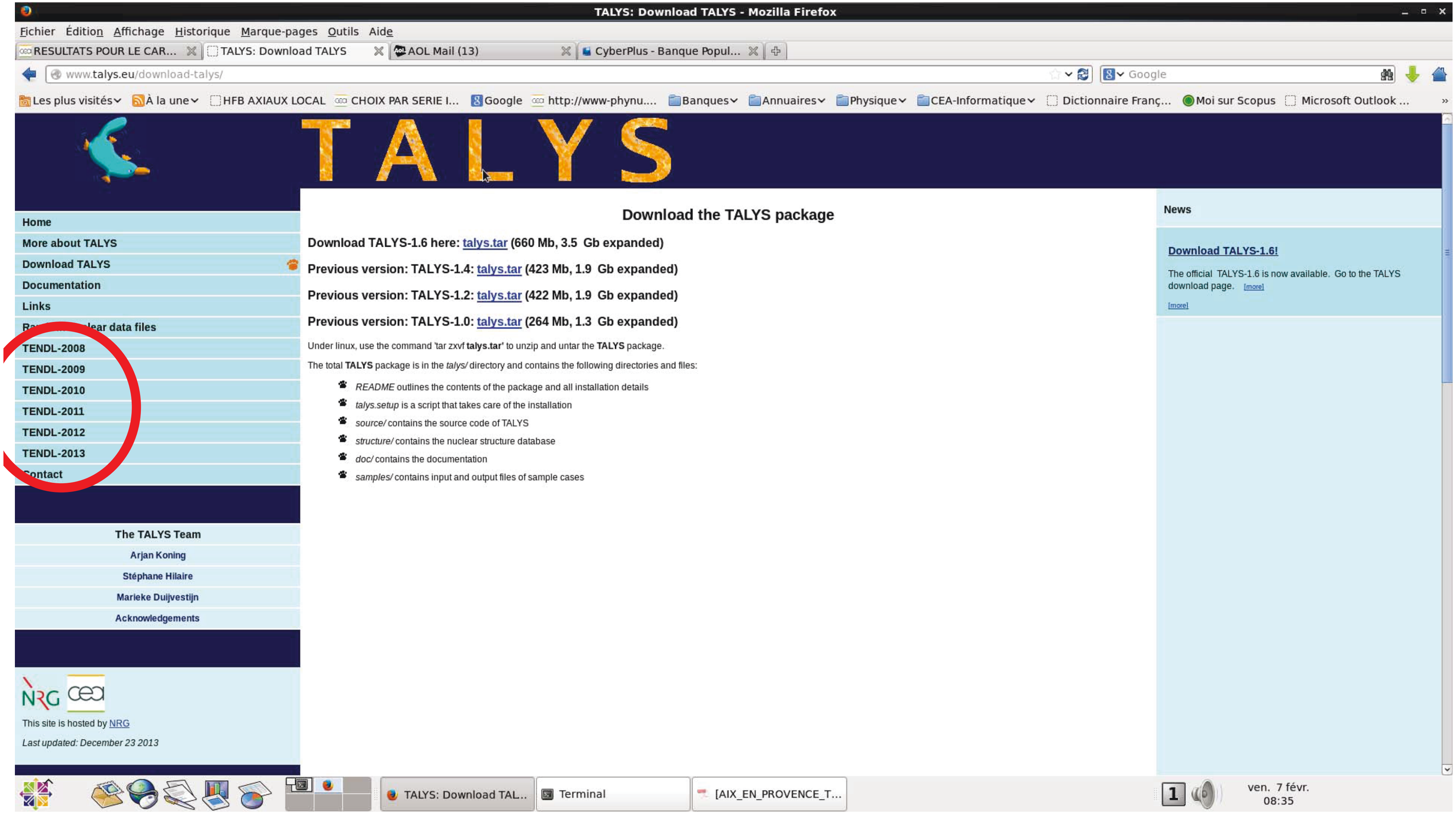
- Neutron, proton, deuteron, triton, Helium-3, alpha and gamma libraries: ENDF-6 format and x-y tables
- 2430 targets (all with lifetime > 1 sec.)
- Neutron library: complete covariance data
- For all nuclides processed MCNP-libraries ("ACE-files") (n,p and d), PENDF files and processed multi-group covariances (neutrons only)

Strategy:

- Always ensure completeness, global improvement, production time: 2 months for 150 processors
- Extra effort for important nuclides, especially when high precision is required (e.g. actinides): Fitted model calculations and direct inclusion of experimental/evaluated data. Keep the input files.
- **All libraries are always reproducible from scratch**
- **All libraries based on compact reaction info:** default TALYS input file or input file with adjusted parameters, parameter uncertainties, resonance parameters + uncertainties, "rescue" file with adoption from other libraries
- Started with 350 nuclei (2008), now 2600 (2014)

# TENDL
# Talys Evaluated Nuclear Data Library (2/2)

## http://www.talys.eu



## Conclusions

- TALYS Fortran-95/2003 upgrade in two phases:
  - 2013: standard issues (arrays, output, etc.)
  - 2014: advanced issues (derived data types, OOP, etc.)
  - Huge computation time decrease targeted for multiple Hauser-Feshbach decay
- Catch up on the TENDL delay
- Couple TALYS with GEF (Schmidt, Jurado) for fission yields, nubar, fission neutron spectrum
- Further develop Total Unified Monte Carlo
- Apply automatic optimization to integral benchmarks for all nuclides
- Extend Total Monte Carlo uncertainty propagation to full core reactor calculations

# Generally speaking prospects

- Nuclear reaction modeling complex and no yet fully satisfactory

  ⇒ pre-equilibrium phenomenon must be improved

  ⇒ fission related phenomena (fission, FF yields & decay) must be improved

- Formal and technical link between structure and reactions has to be pushed further

  ⇒ pre-equilibrium and OMP efforts already engaged

  ⇒ computing time is still an issue

- Fundamental $\nu$-$\nu$ interaction knowledge (and treatment) has to be improved

  ⇒ Ab-initio not universal (low mass or restricted mass regions)

  ⇒ Relativistic aspects not included systematically

  ⇒ Human & computing time is still an issue

# TALYSly speaking prospects

- TALYS Fortran-95/2003 upgrade
- Couple TALYS with GEF (Schmidt, Jurado) for fission yields, nubar, fission neutron spectrum
- Further develop Total Unified Monte Carlo
- Apply automatic optimization to integral benchmarks for all nuclides
- Extend Total Monte Carlo uncertainty propagation to full core reactor calculations
- Include or (couple to) new models