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TALYS: A unified approach towards nuclear reaction calculations

Arjan Koning[1,2]

[1]Division of Applied Nuclear Physics, Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

[2]Nuclear Research and Consultancy Group (NRG), Petten, The Netherlands

Email: koning@nrg.eu

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Outline

- Introduction to the TALYS code
- Today's examples:
  - Fission cross sections and yields
  - Residual production cross sections
  - Astrophysics: Solar abundances
- Parameter uncertainties and links to applications
- Summary

TALYS

- Nuclear model code by NRG Petten, CEA Bruyeres-le-Chatel, UL Bruxelles
- g,n,p,d,t,h,a induced reactions from 10^{-5} eV up to 250 MeV

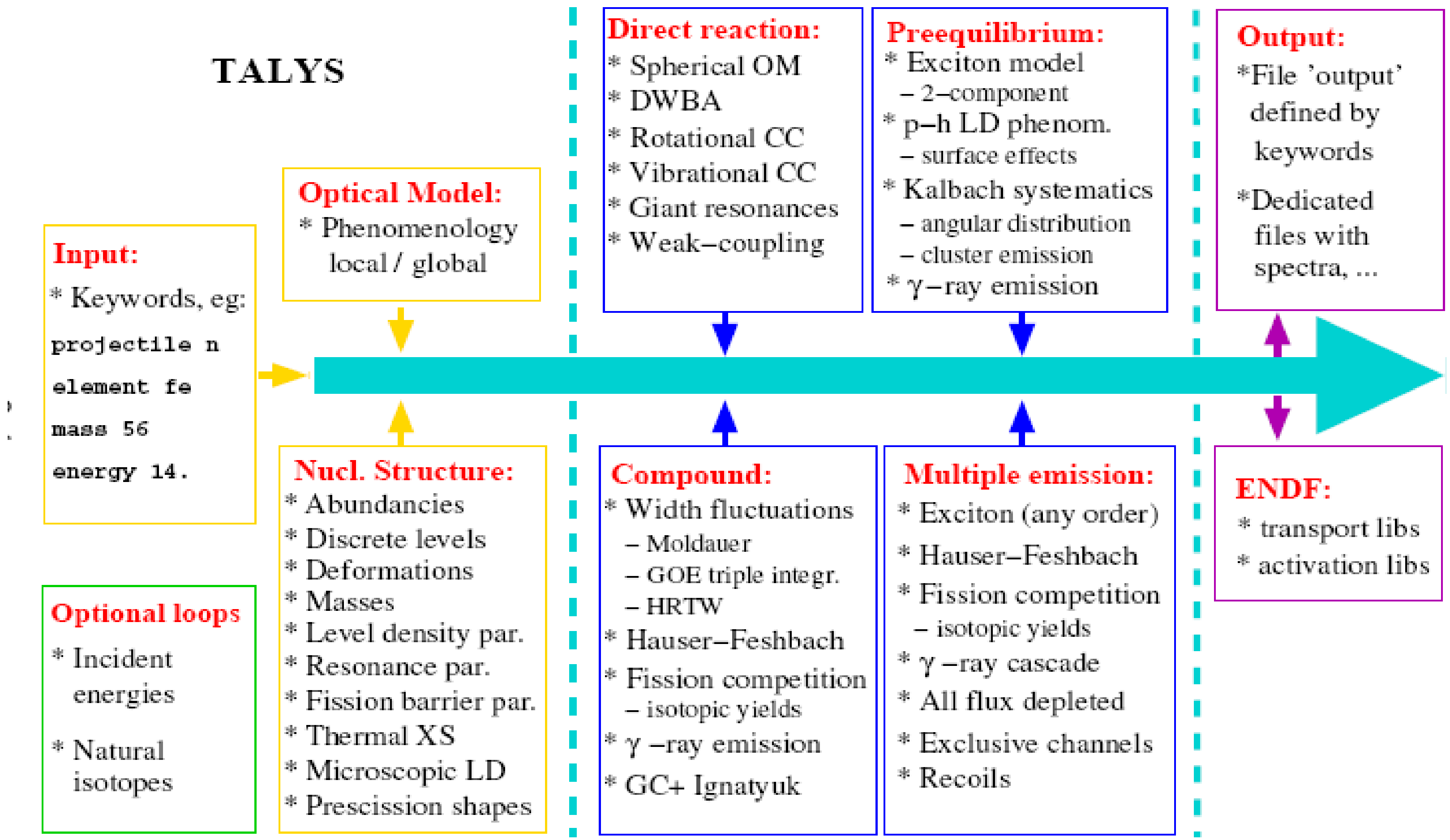
Release:

- www.talys.eu
- Latest official version, TALYS-1.6, released december 21, 2013.
- Estimated 500-1000 users, > 800 publications

Software issues:

- TALYS is ready to be used by persons other than the authors
- Very flexible:
  - 4-line idiot-proof input (element, mass, projectile, energy), but also...
  - > 250 keywords to change models, parameters, level of output, etc.
- 300 page manual, 20 widely varying sample cases
- Readable modular programming (extensions by others is relatively easy)
- Very robust, thanks to dripline-to-dripline and random input testing

TALYS code scheme



TALYS physics

General use:

- TALYS can be used for

  In-depth single nuclide/reaction analyses

  Global multi-nuclide calculations

Complete output:

- Total, partial and residual production cross sections, (Double)-differential spectra, Angular distributions per discrete level, Fission yields, Recoils, Isomeric production, Astrophysical reaction rates Gamma production, etc,

Recent accomplishment: option to use all optical, level density, fission and pre-equilibrium models phenomenological (Woods-Saxon, Fermi gas, Hill-Wheeler, exciton) or microscopical (Hartree-Fock-Bogolyubov-based, by Hilaire, Goriely, Bauge)

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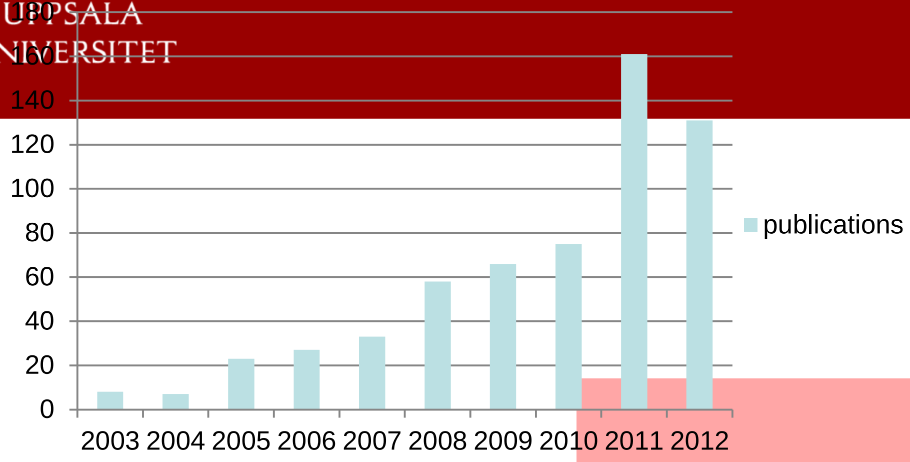
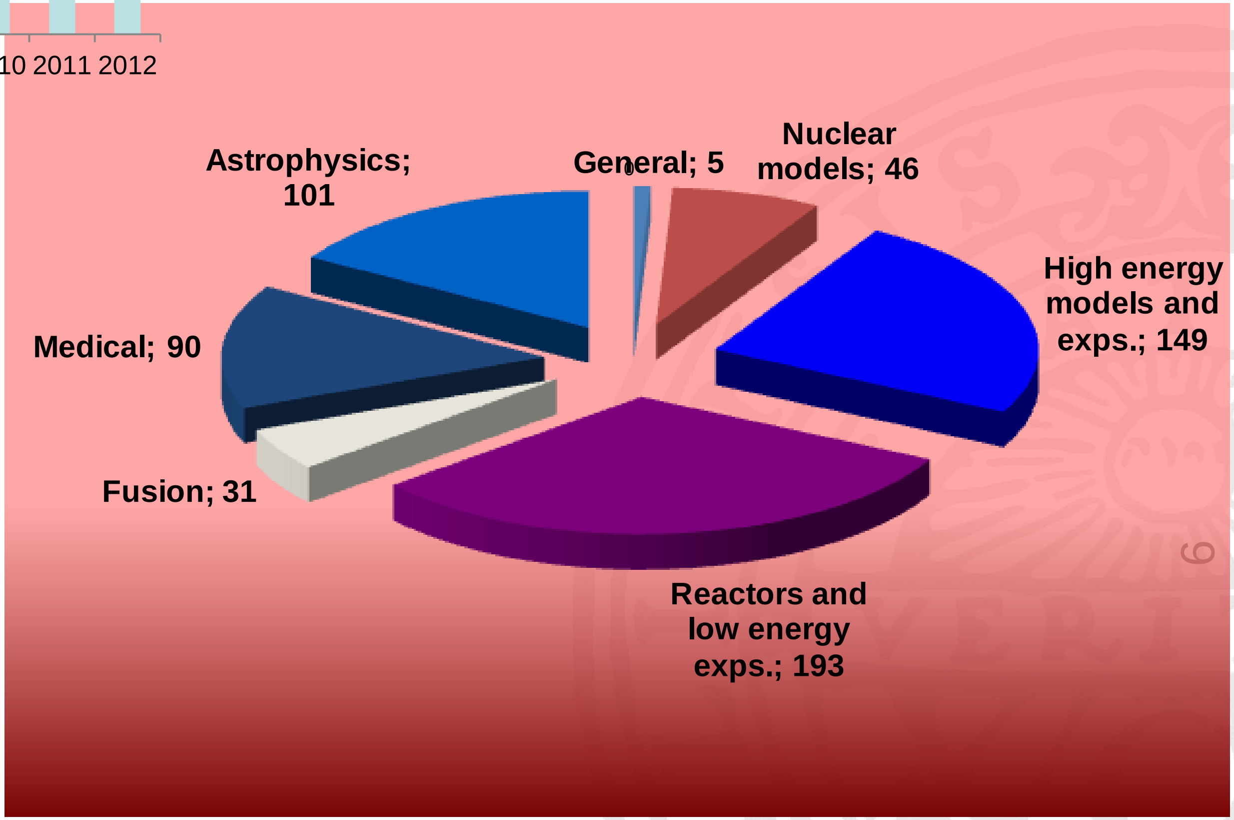
TALYS publications





Non statistical effects in nuclear level densities (HFB + D1S Gogny)

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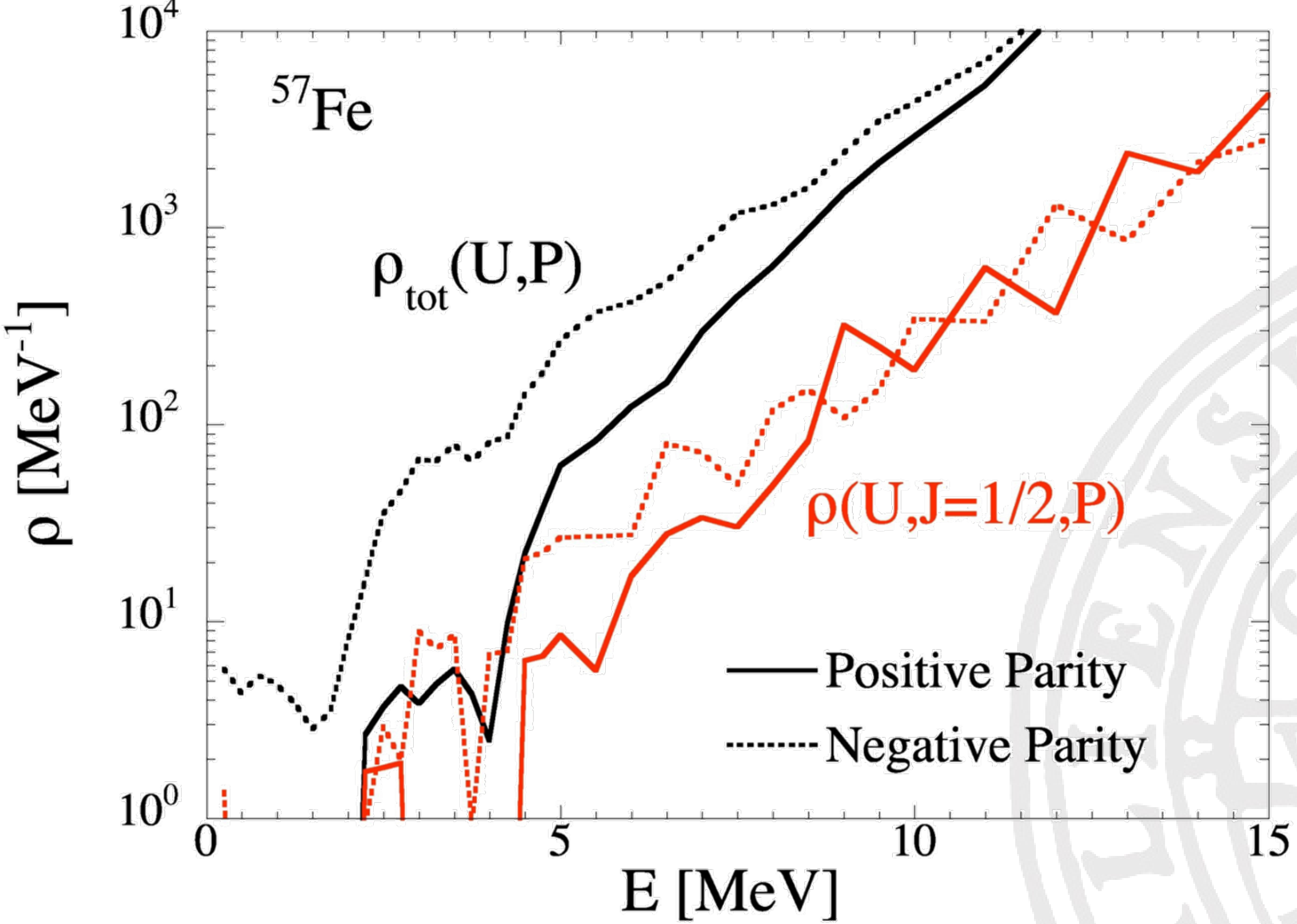
Talys deals with realistic (non statistical) spin & parity distributions



Non statistical effects in nuclear level densities

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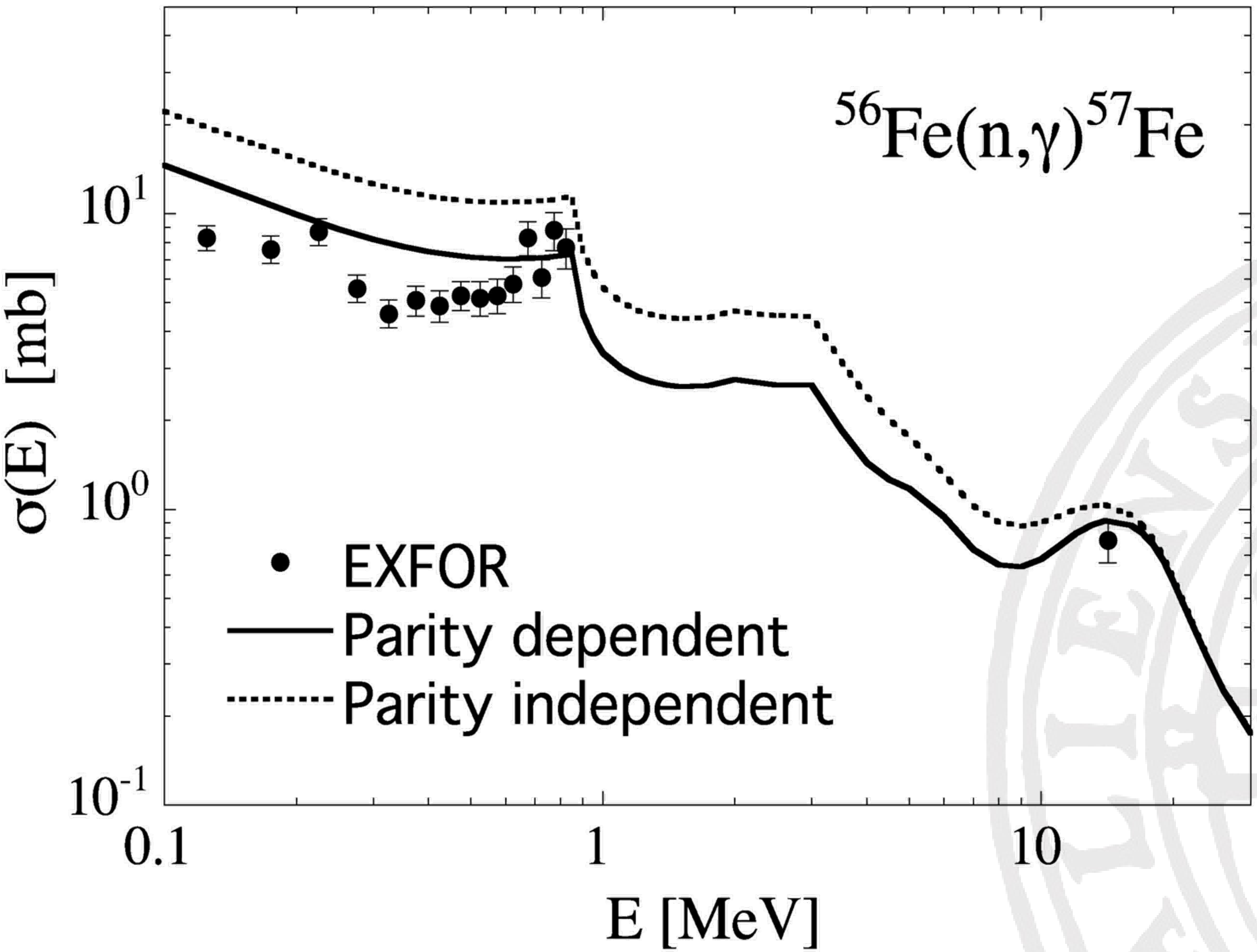
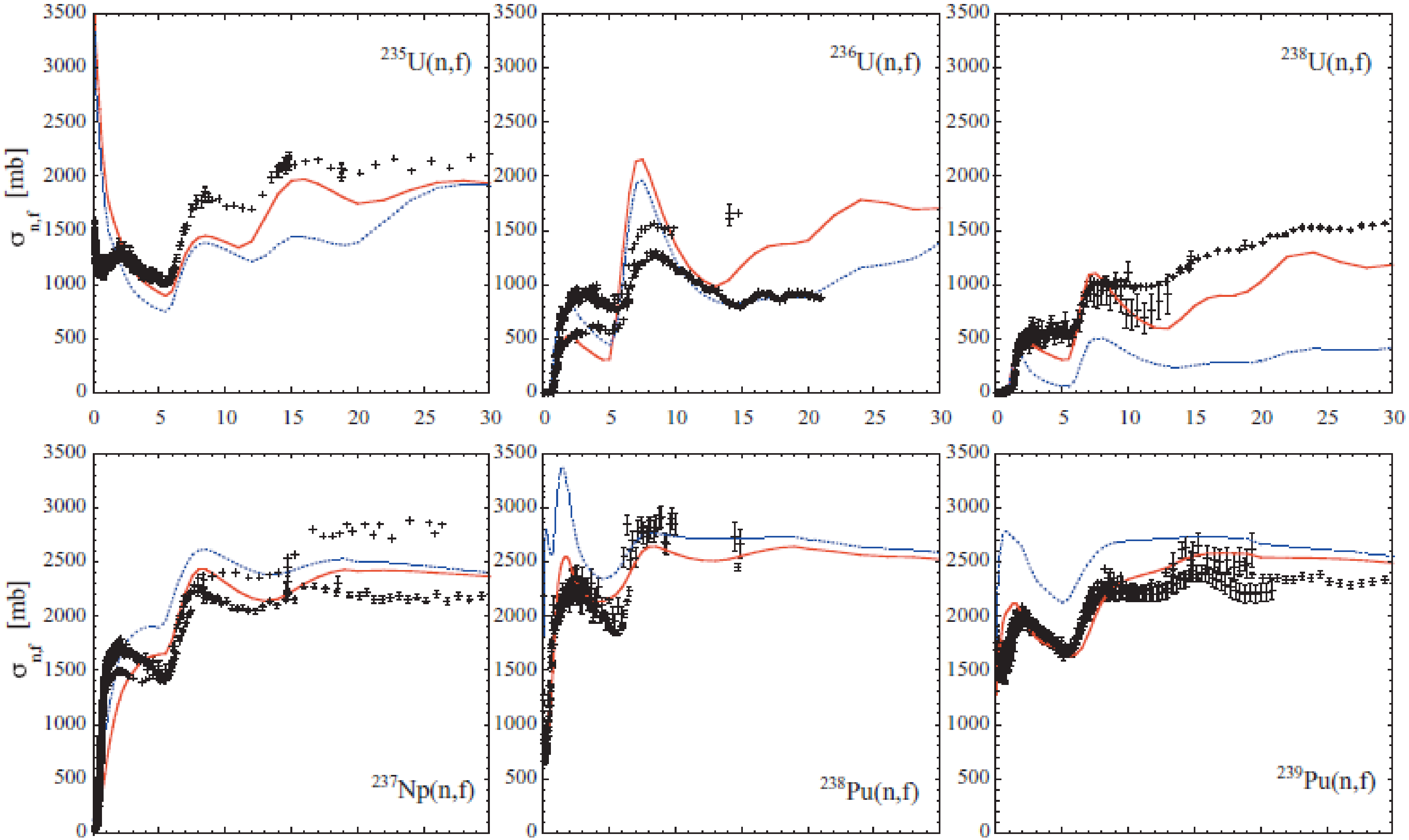


TALYS: Microscopic fission



S. Goriely, S. Hilaire, A.J. Koning, M. Sin and R. Capote, Phys Rev C79, 024612 (2009)

TALYS: Phenomenological fission

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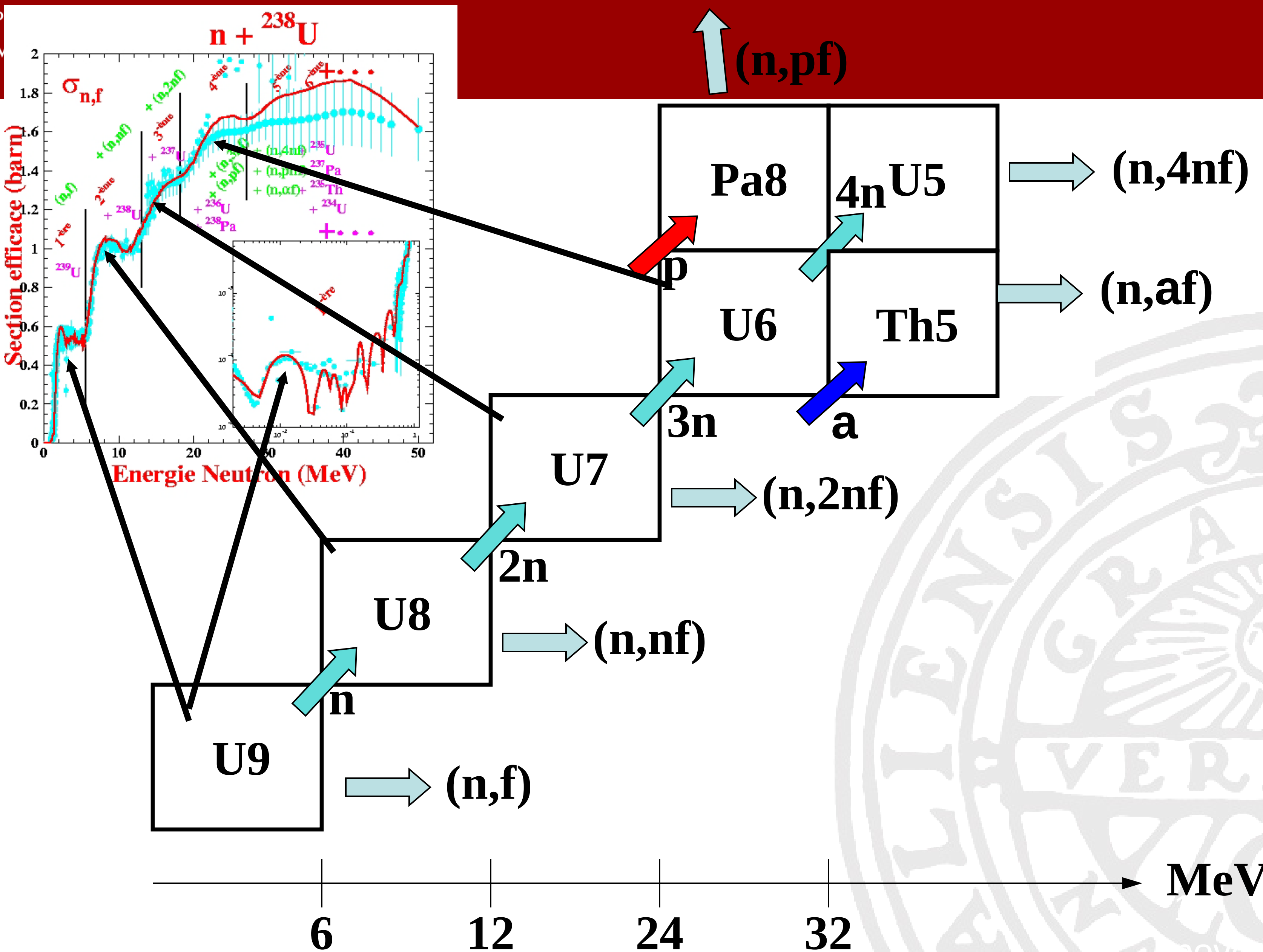
Coherent fission cross sections with phenomenological approach

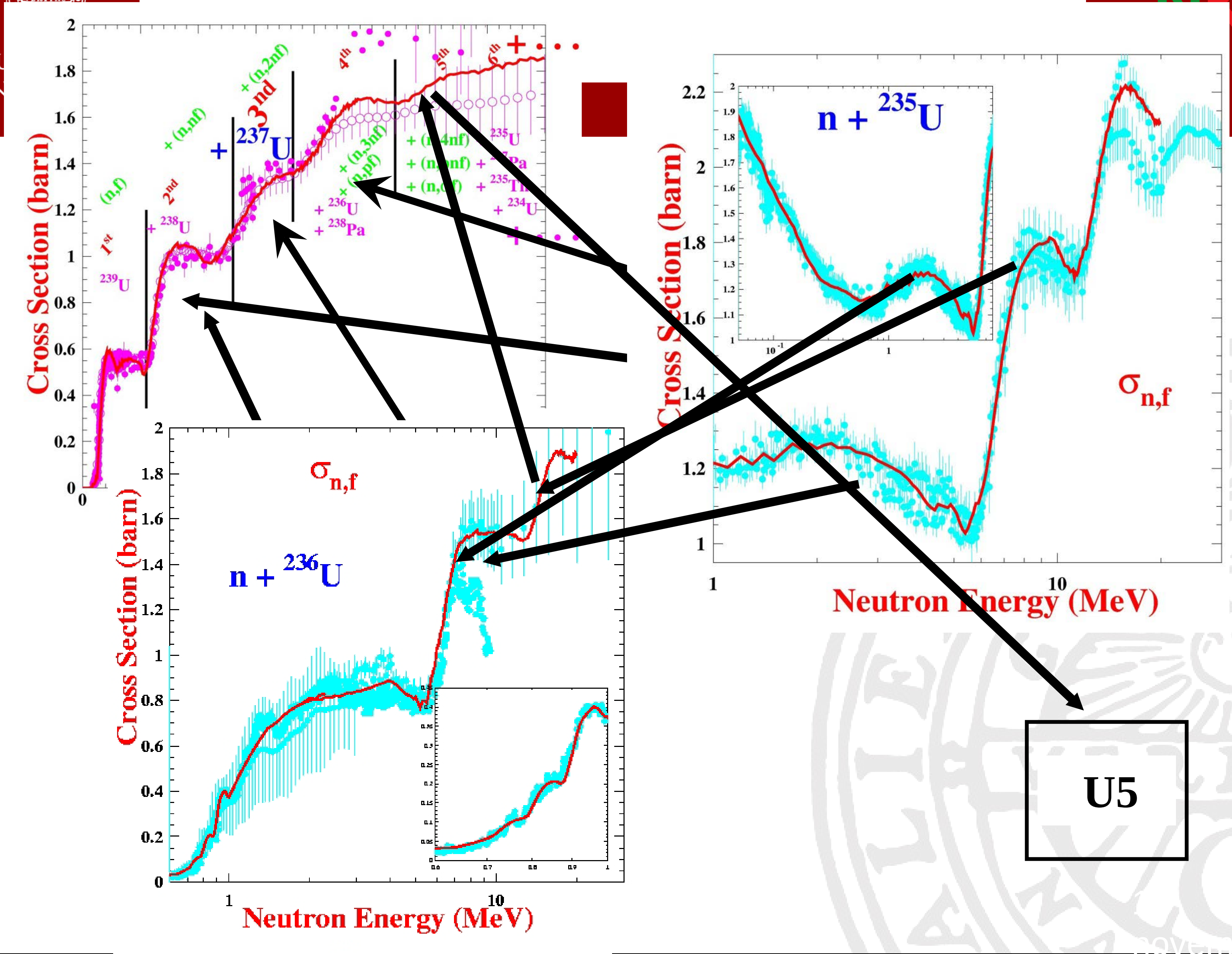
Neutron induced fission on ^{238}U

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

TALYS: phenomenological fission

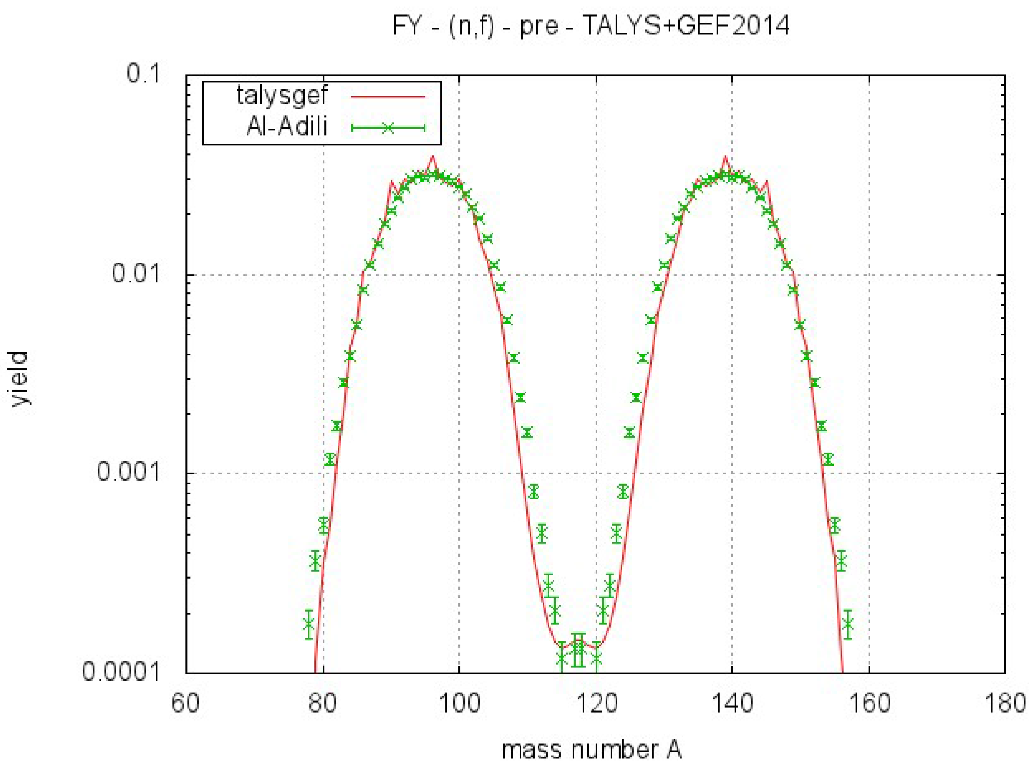


TALYS: Phenomenological fission



Fission yields

- **TALYS is now coupled with GEF, a fission code by Karl-Heinz Schmidt (GSI), which calculates fission observables on a microscopic basis, starting from an excitation energy, spin and parity**
- **TALYS feeds GEF with that starting point**



$^{234}U(n,f)$

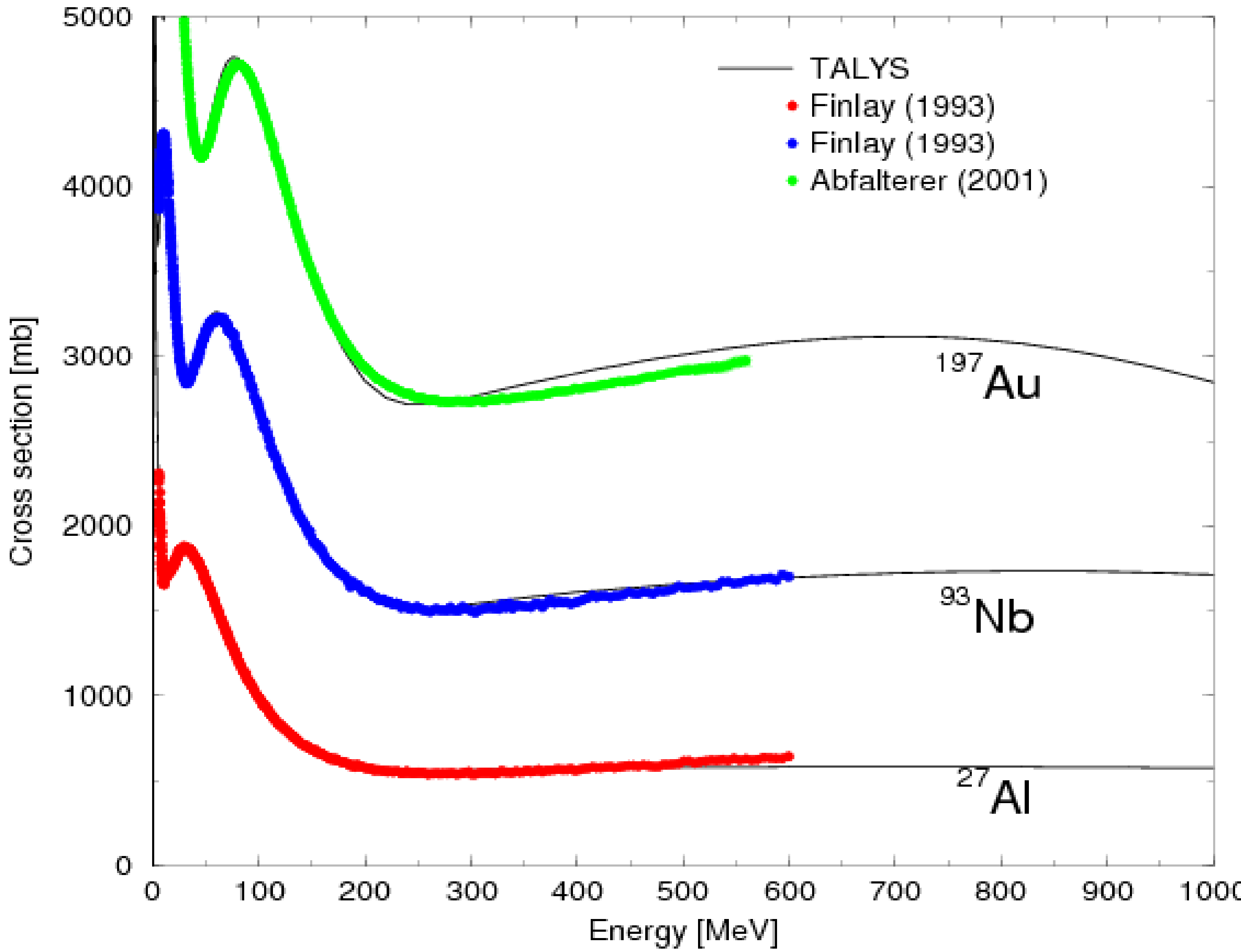
Experimental data from PhD thesis of Ali Al-Adili, Uppsala University 2013.

More examples: S. Pomp Presentation at FIESTA 2014, Santa Fe

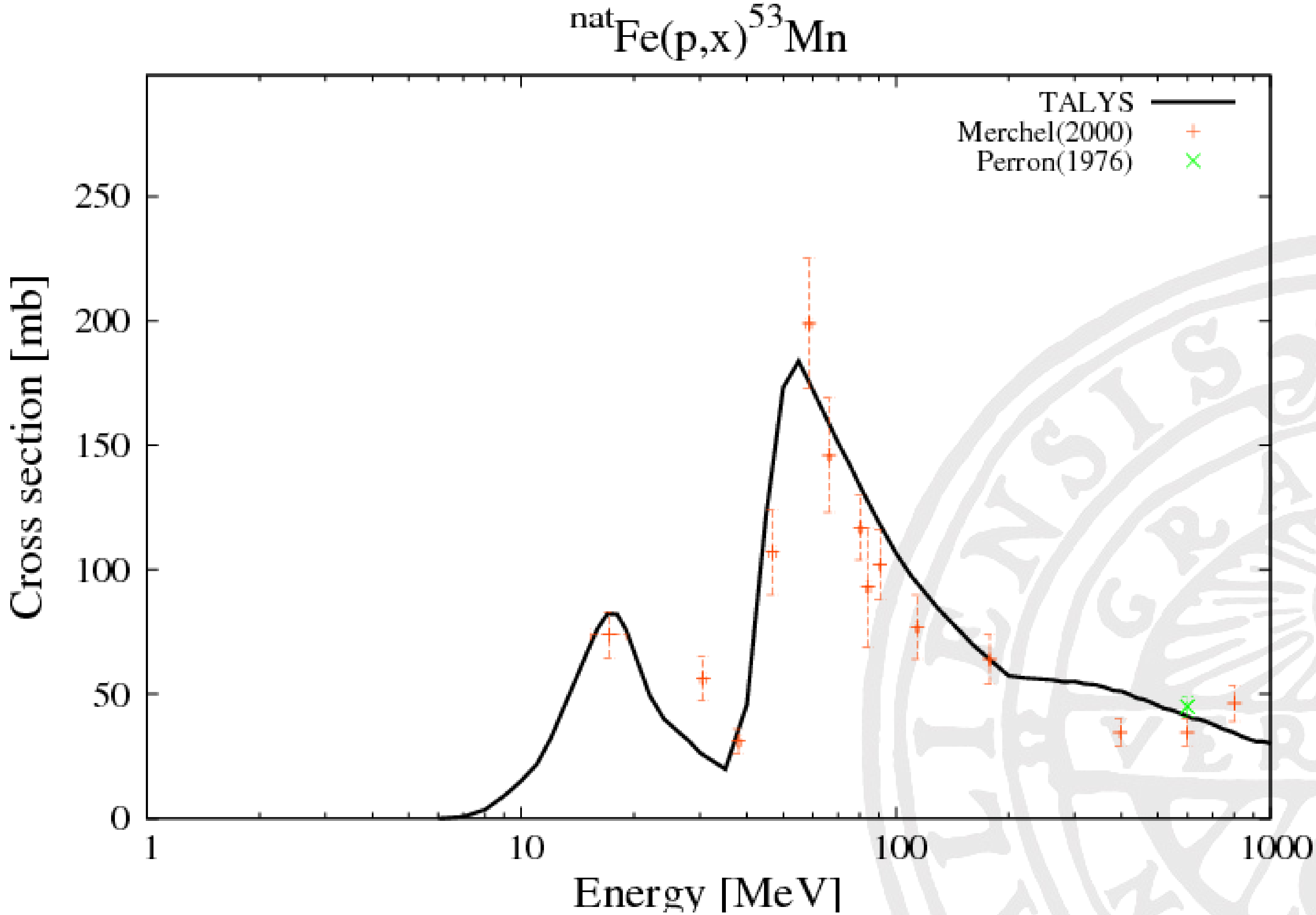
"Formal" (computational) extension to 1 GeV

- Extension of KD03 OMP to higher energies: smooth extension of Vv(E) to negative values, double increase of Wv(E) above 200 MeV (ND2013)
- Exciton model for pre-equilibrium reactions: multiple pre-equilibrium emission up to any order already in TALYS, exciton model works at higher energies (see e.g. Mashnik-CEM, Chadwick-Hybrid MC).
- New mechanisms – Pion prediction and fragmentation: Not (yet) taken into account, at which energy do we pay the price?
- Multiple Hauser-Feshbach decay: Equidistant excitation energy grid no longer appropriate. Logarithmic grid introduced for all residual nuclides in the reaction chain.
- TALYS-1.6
  - Total and residual production cross sections tested to some extent
  - Spectra and angular distributions not tested
  - Which is all acceptable……as long as the code doesn't crash!
  - Gives user more flexibility to switch from a high-energy (INC) code to TALYS

Neutron total cross section

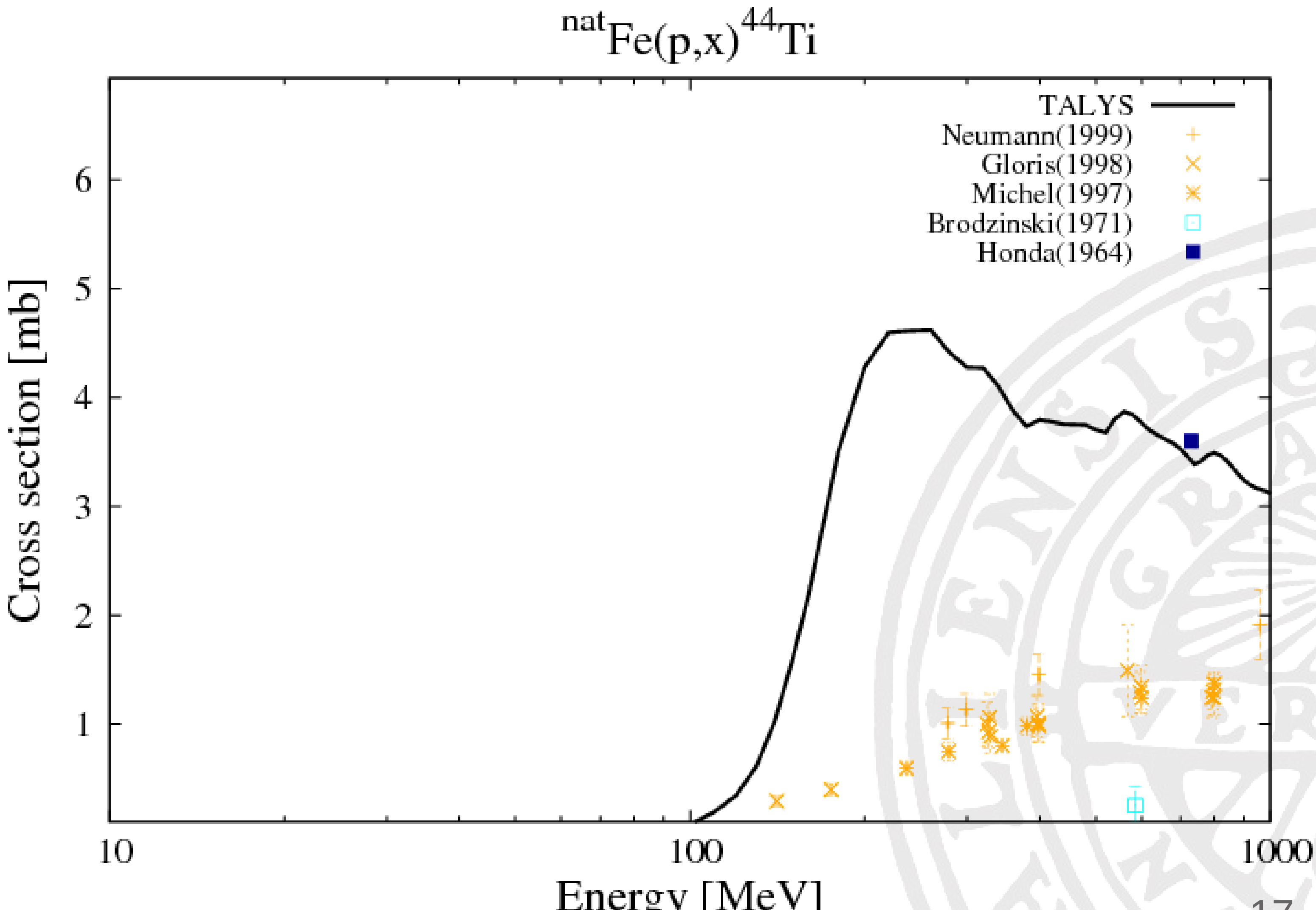


Fantastic!



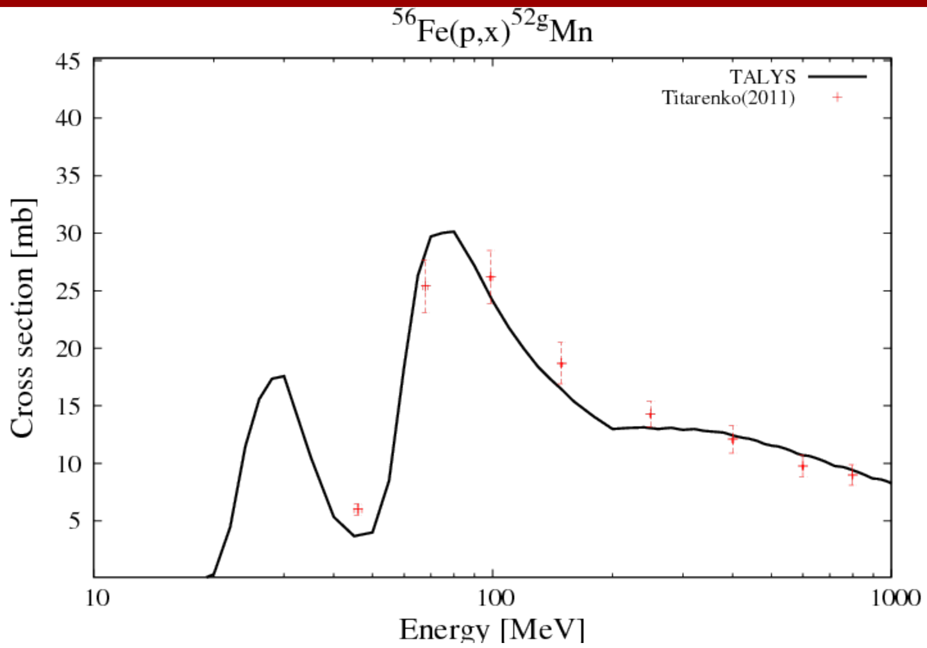
natFe(p,x)53Mn
TALYS
Merchel(2000)
Perron(1976)
Cross section [mb]
250
200
150
100
50
0
1
10
100
1000
Energy [MeV]

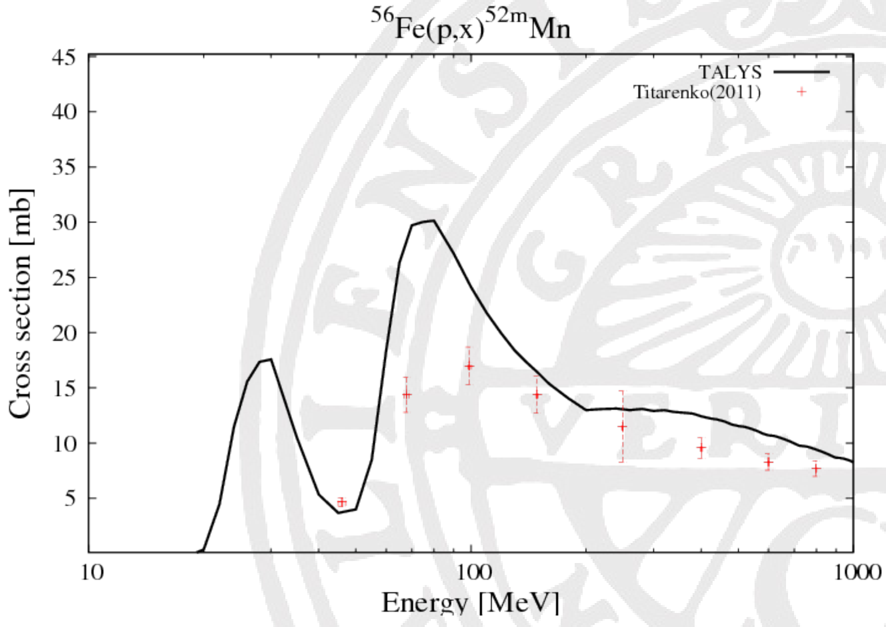
Awful!



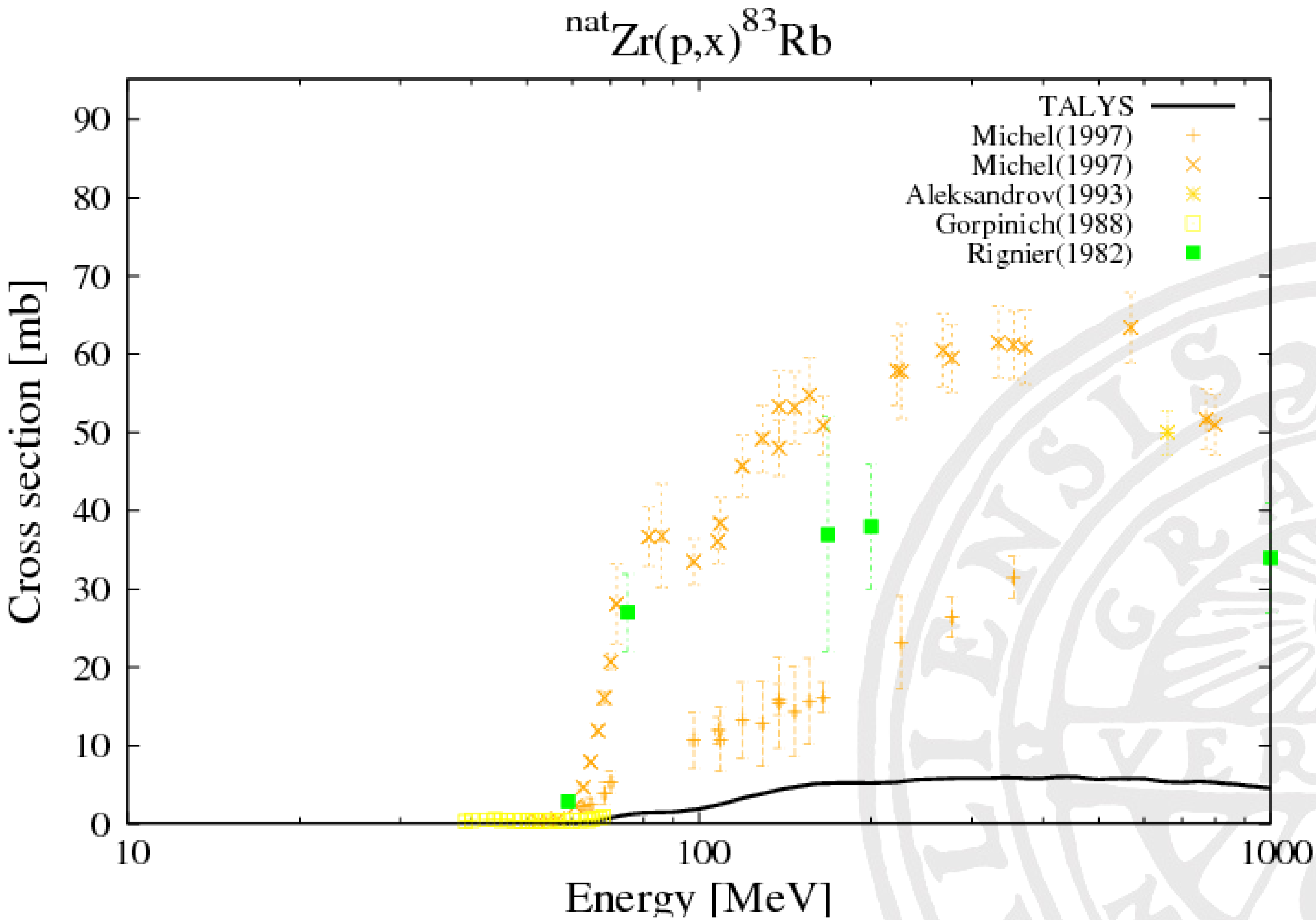
natFe(p,x)44Ti
TALYS
Neumann(1999)
Gloris(1998)
Michel(1997)
Brodzinski(1971)
Honda(1964)
Cross section [mb]
1
2
3
4
5
6
10
100
1000
Energy [MeV]

Not bad at all!



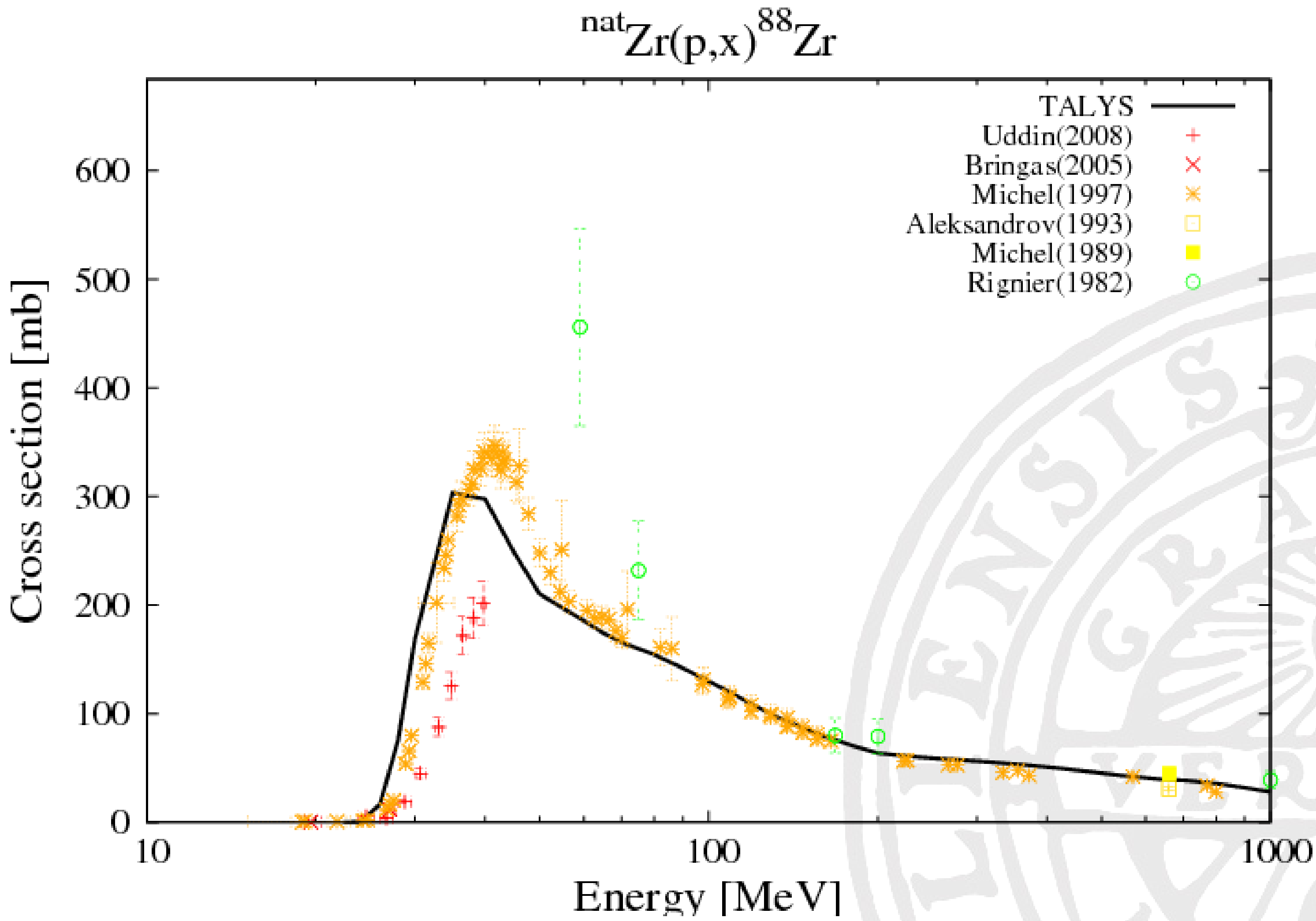


Terrible!



$^{nat}Zr(p,x)^{83}Rb$
TALYS
Michel(1997)
Michel(1997)
Aleksandrov(1993)
Gorpinich(1988)
Rignier(1982)
Cross section [mb]
Energy [MeV]
0
10
20
30
40
50
60
70
80
90
10
100
1000

And finally: rather good!



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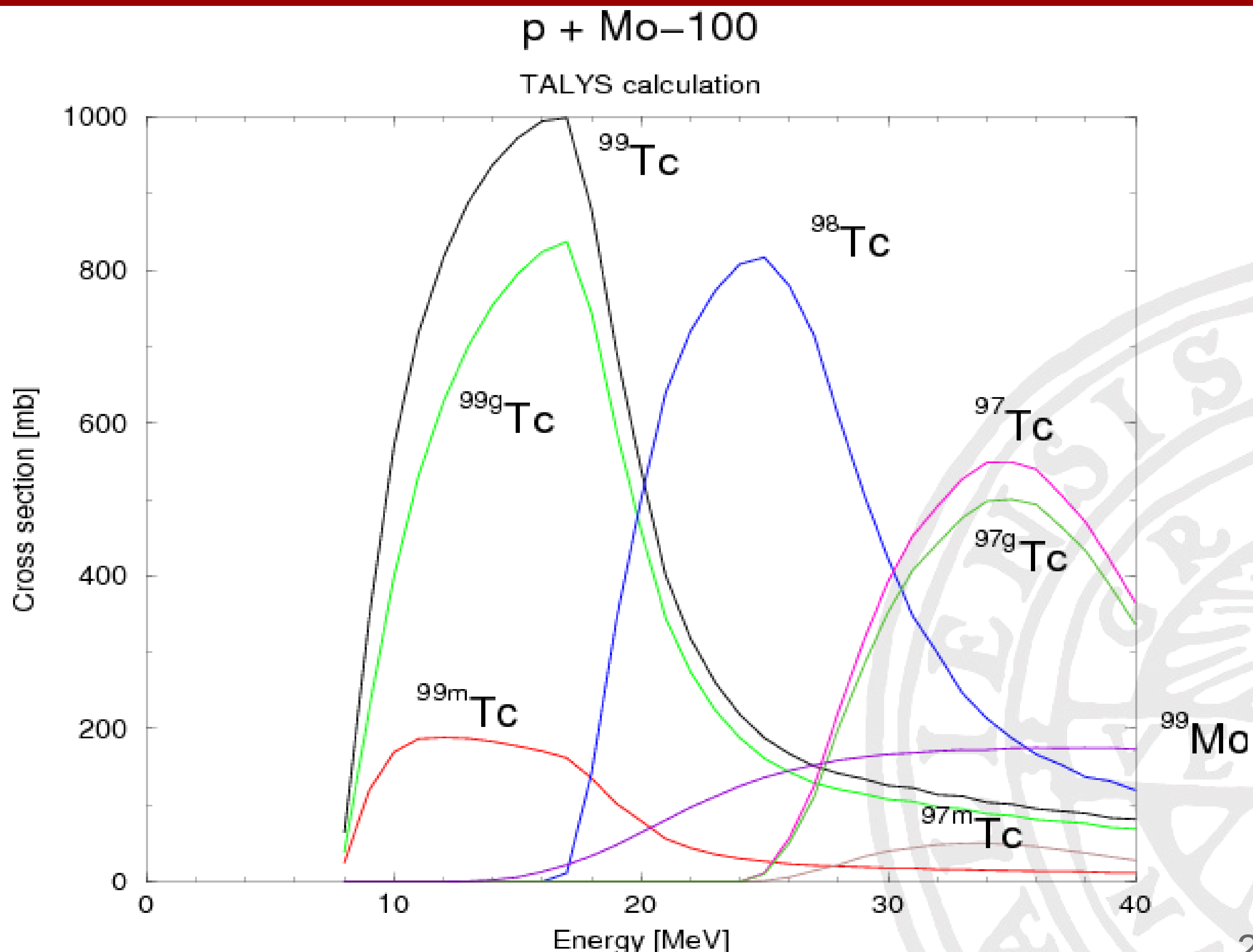
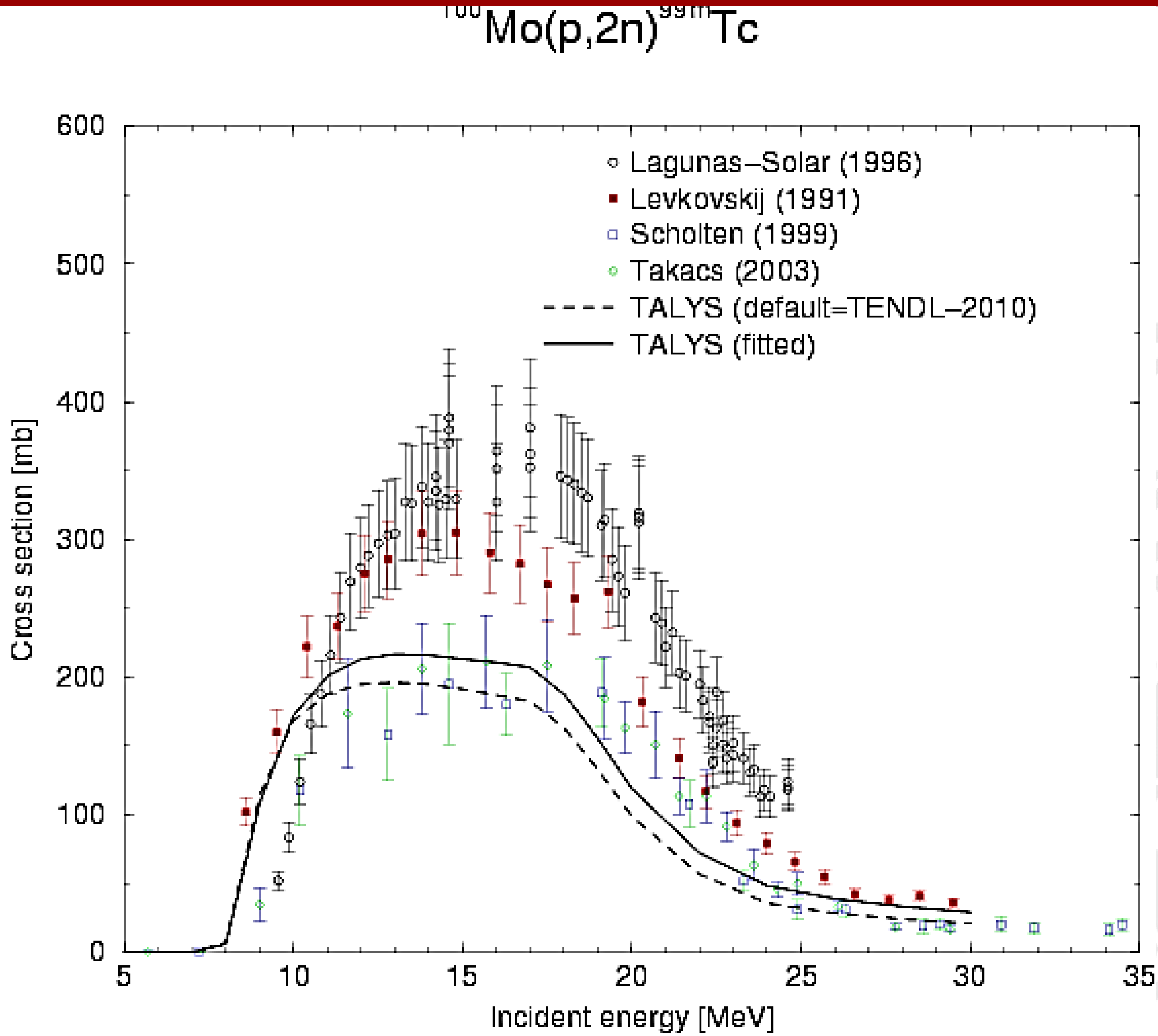
Medical isotope production



Medical isotope production



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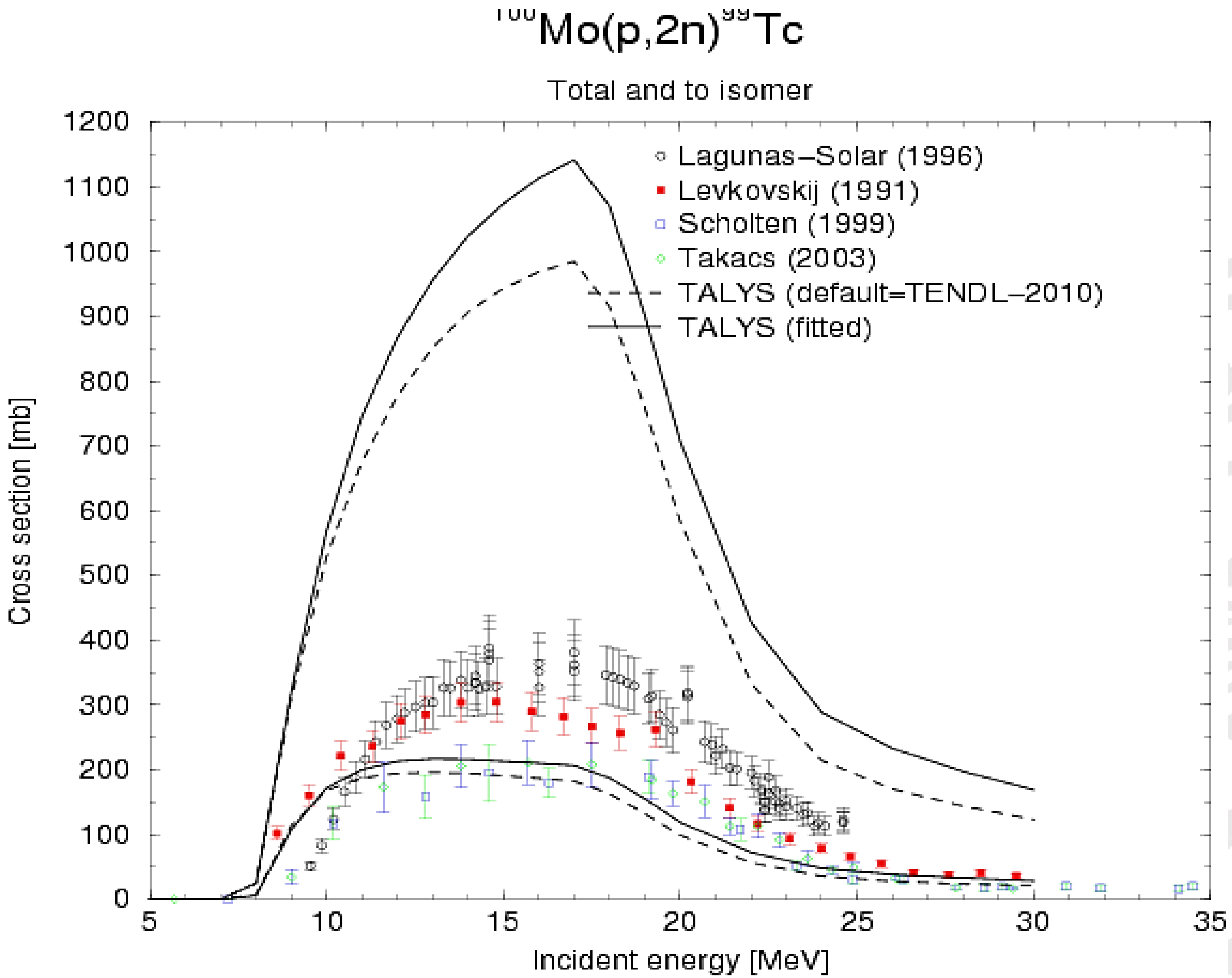
Isomeric ratio is essential: about 0.22!



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

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

Two options :

- Supernovae :

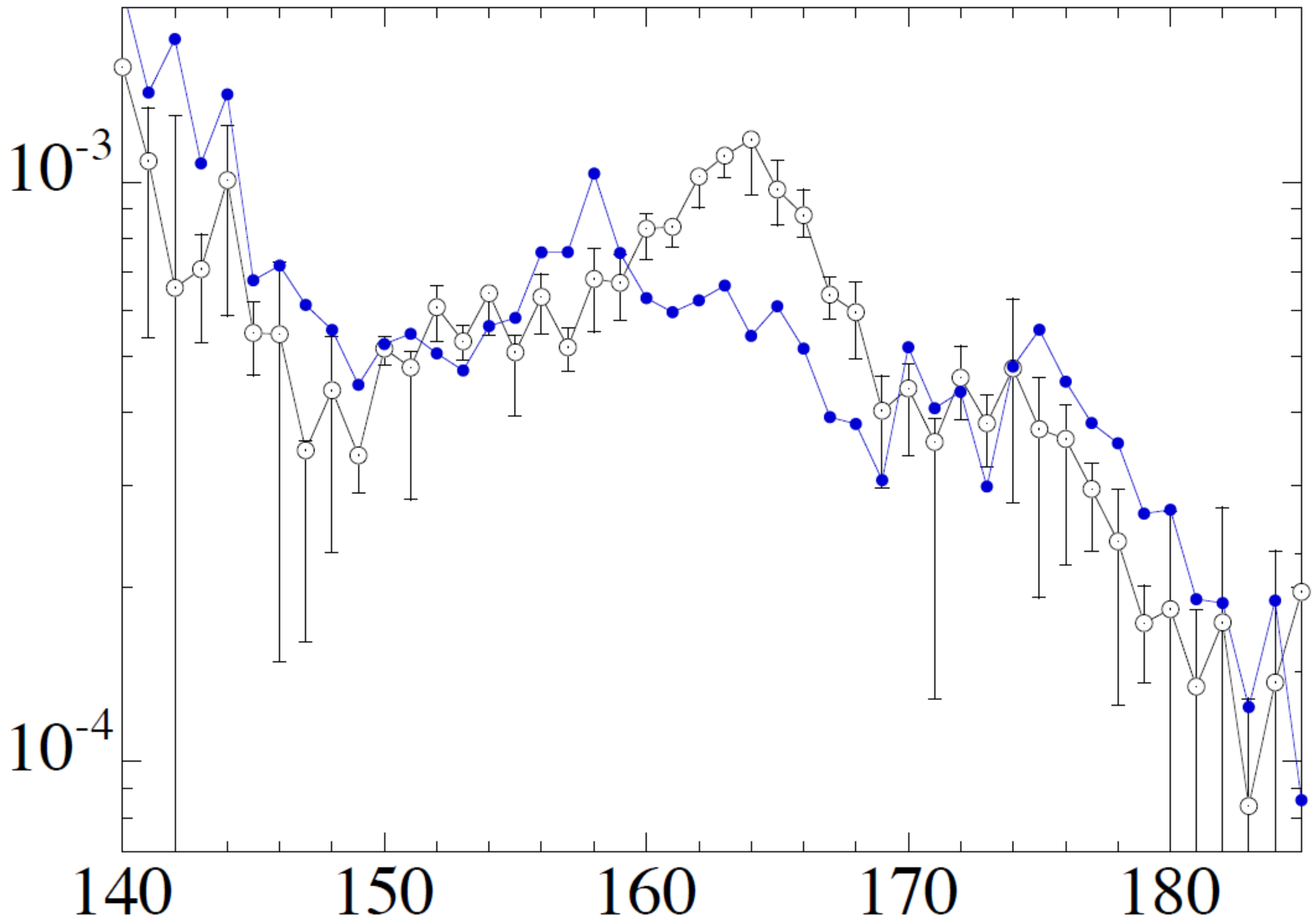
Matter ejection without any problem		+++
Great sensitivity to thermodynamical conditions		- - -
No clearly identified astrophysical site		- - -
Failure of explosion models		- - -

- Neutron stars collisions :

Enough neutrons		+++
Binary systems abundancies ?	**Recently solved**	+++
Matter ejection ?		- - -
Large sensitivity to fission models		- - -

GLOBAL SYSTEMATIC APPROACHES
Astrophysical r-process (2/4)

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



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

Binary systems hydrodynamic

AMEDEE (HFB+D1S)

Fission fragment yields

r-process nucleosynthesis

TALYS

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

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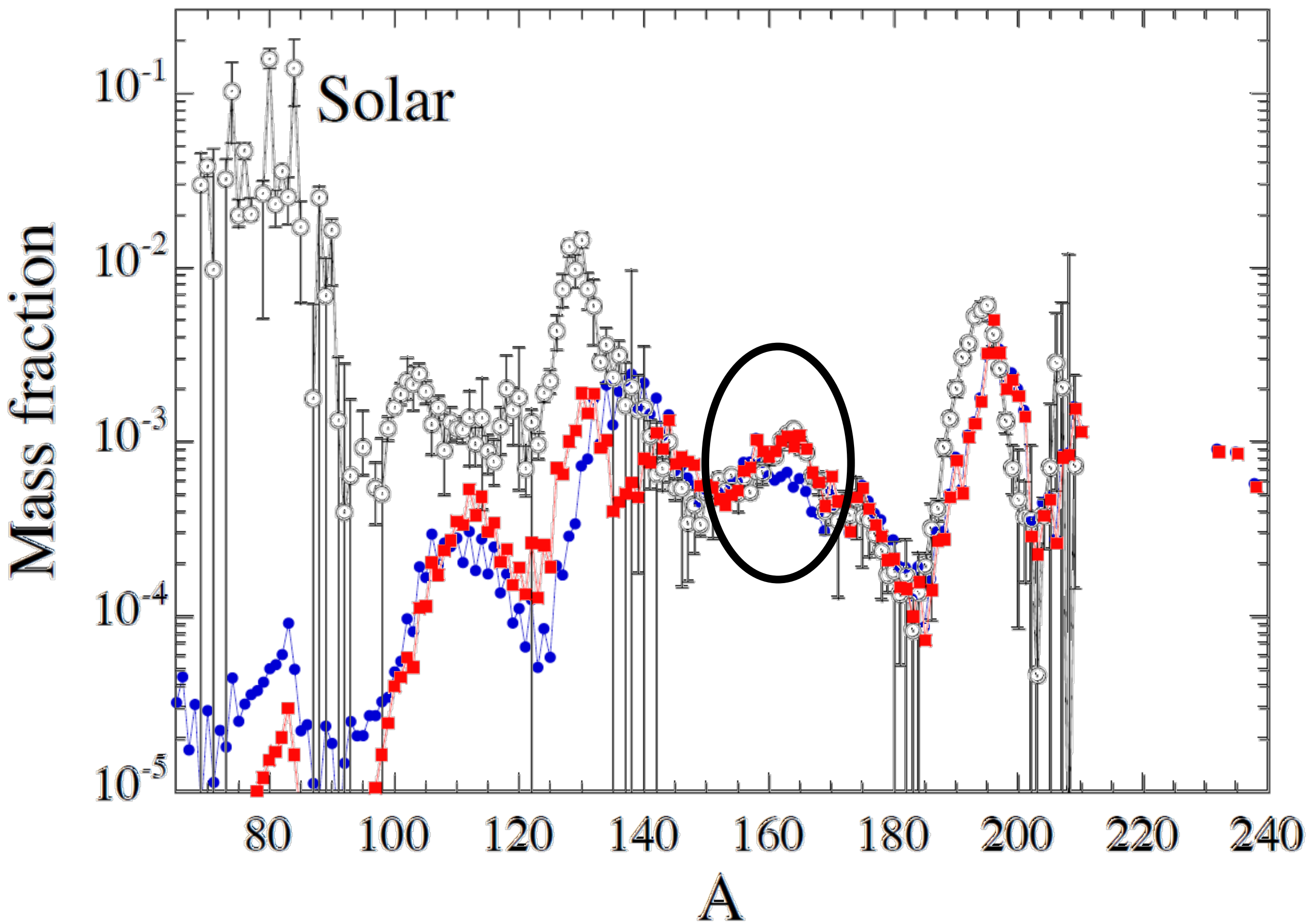
Solar abundancies for 140 ≤ A ≤ 200 : situation before 2013 ?

Solar abundancies for 140 ≤ A ≤ 200 : situation in 2013



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

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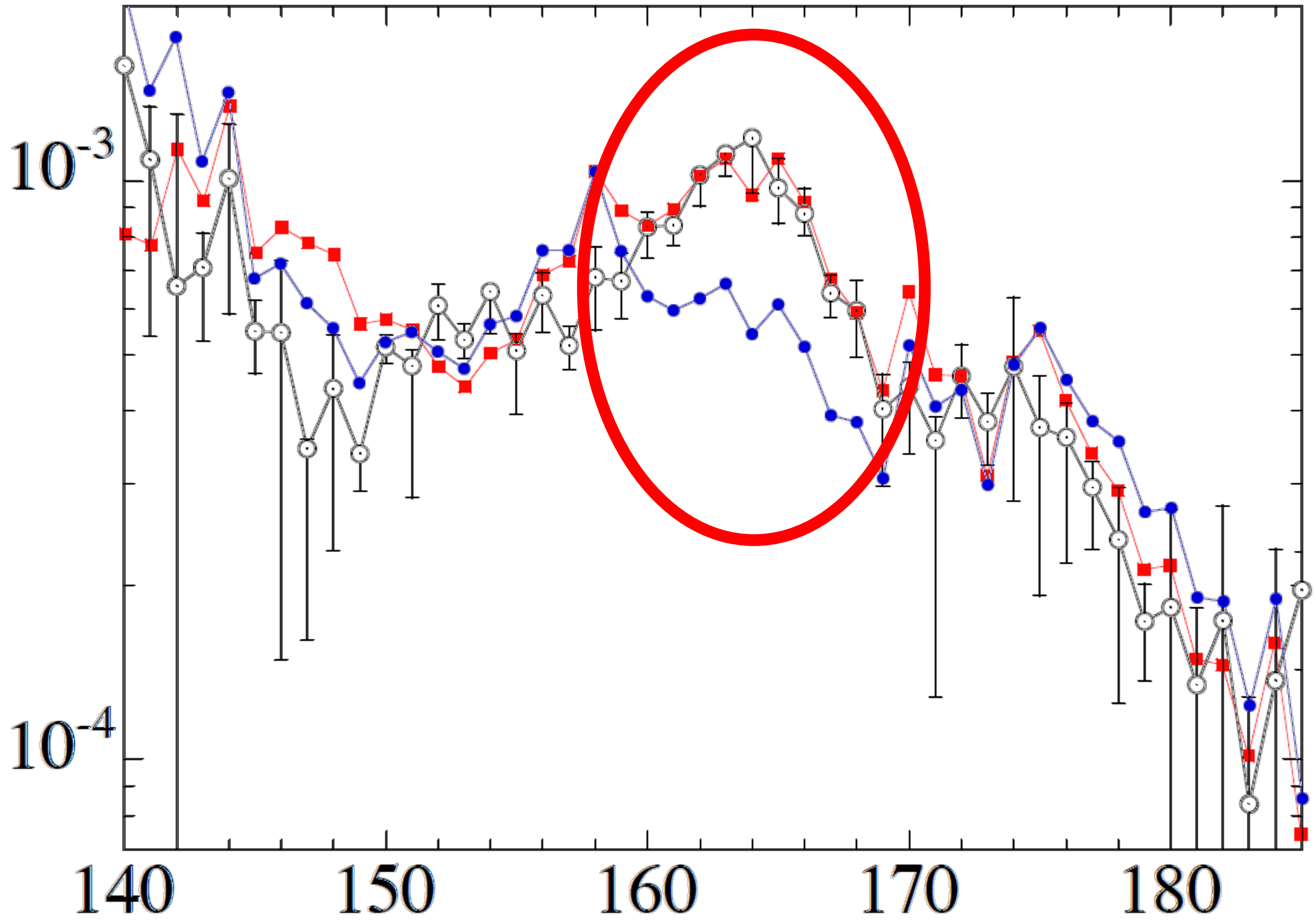


More details for discussions/explanations in Goriely et al, PRL 111, 242502 (2013)

Covariances from nuclear model calculations

Experimentalists:

- are well educated: give uncertainties with their results.

Theoreticians:

- Bad behaviour: most of them say their models are good (or bad), but none of them says how good (or bad): x-y instead of x-y-dy

No excuse possible:

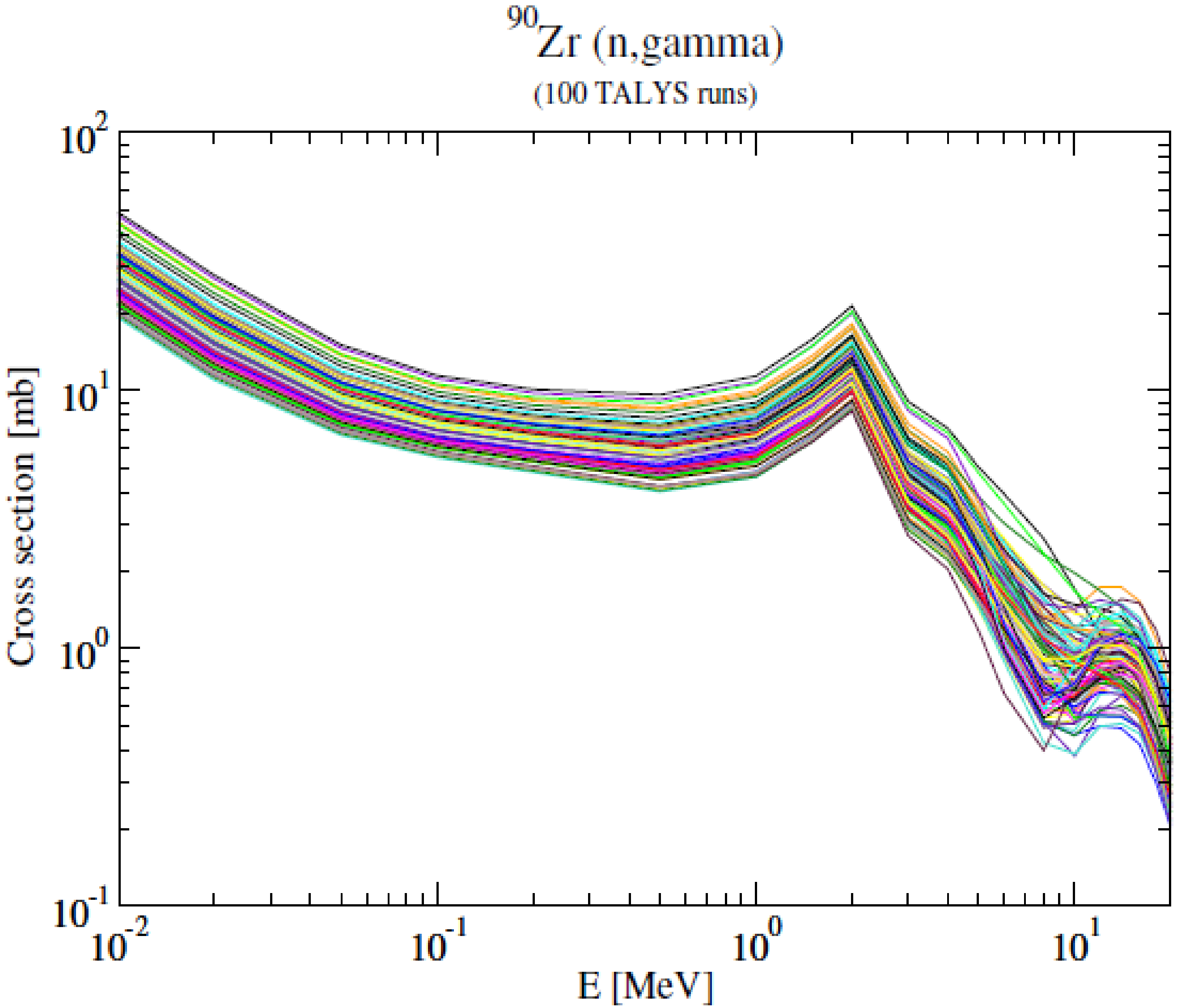
- the strong nucleon-nucleon force is not known,
- the exact many-body problem is not solved,
- $\longrightarrow$ all nuclear models are limited
- so where are the uncertainties of all the cross sections, spectra, angular distributions, etc.?

Approach

- Find a nuclear model code that predicts all open reaction channels, and is very flexible in input and output.
- Assess realistic uncertainties for the input, i.e. nuclear model, parameters.
- Propagate these uncertainties directly to the cross sections, angular distributions, gamma production, energy spectra, etc. using a Monte Carlo method.
- Obtain full covariance matrix (diagonal elements $\longrightarrow$ uncertainties).

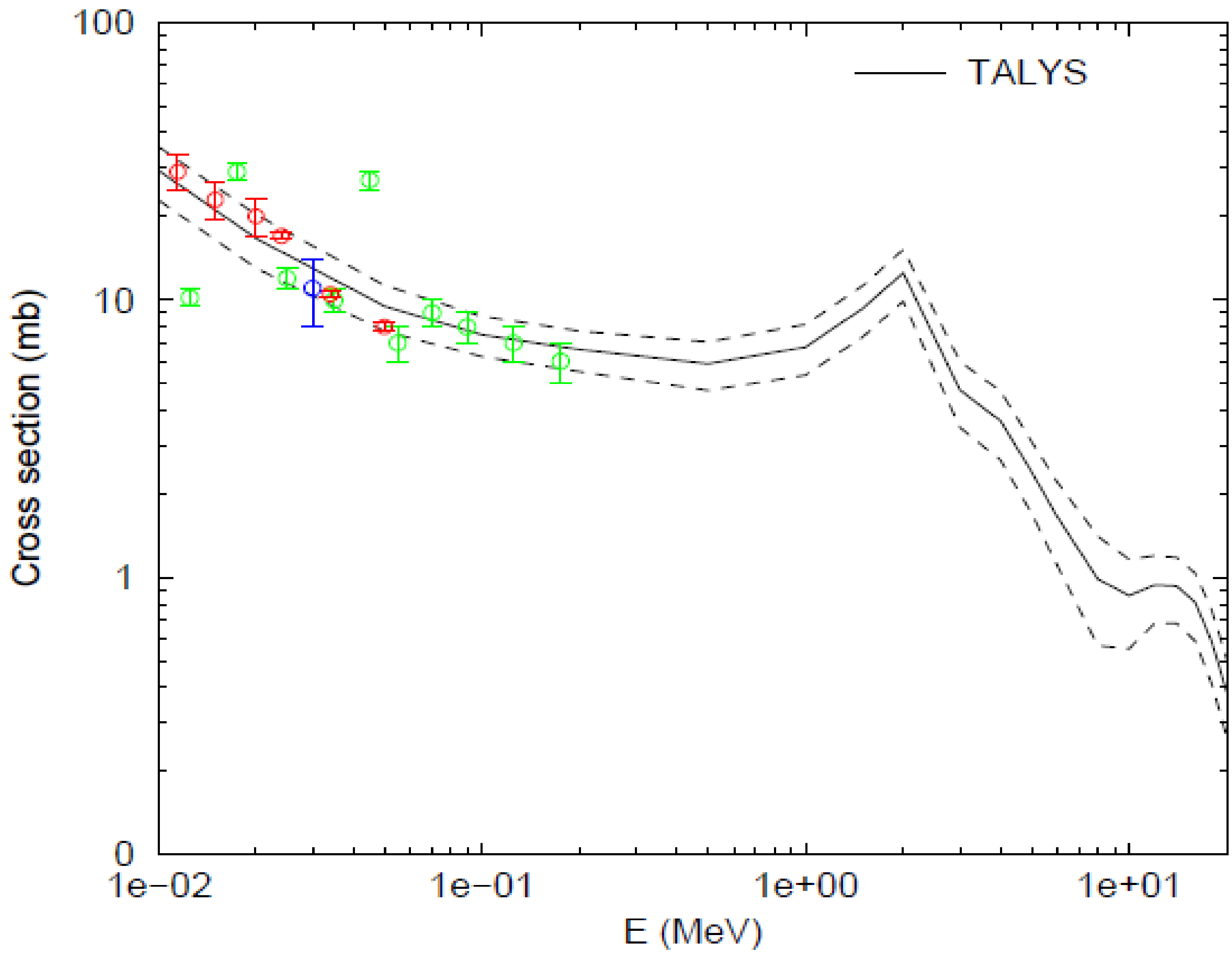
Covariances

- Nuclear model parameter vector **p**: e.g. $p^1 = a_{ld}(26,56)$, $p^2 = a_{ld}(26,57)$, $p^3 = r_V$, etc.
- Physical quantity vector σ of length N: e.g. $\sigma^1 = \sigma_{n\gamma}(E_1), \ldots, \sigma^i = d\sigma_{el}/d\Omega(E_1,\Theta_1), \ldots, \sigma^N$
- $\sigma = T(\mathbf{p})$, where the function T stands for TALYS.
- Let $\mathbf{p}_0, \sigma_0$ be the best parameter/quantity set.
- Perform $k = 1, K$ (=1000) TALYS calculations with p drawn at random from a Gaussian distribution.
- Covariance matrix $V_{ij} = \frac{1}{K}\sum_{k=1,K}(\sigma_k^i - \sigma_0^i)(\sigma_k^j - \sigma_0^j)$ for i,j=1,N
- Relative covariance matrix: $R_{ij} = V_{ij}/(\sigma_0^i \sigma_0^j)$ for i,j=1,N.

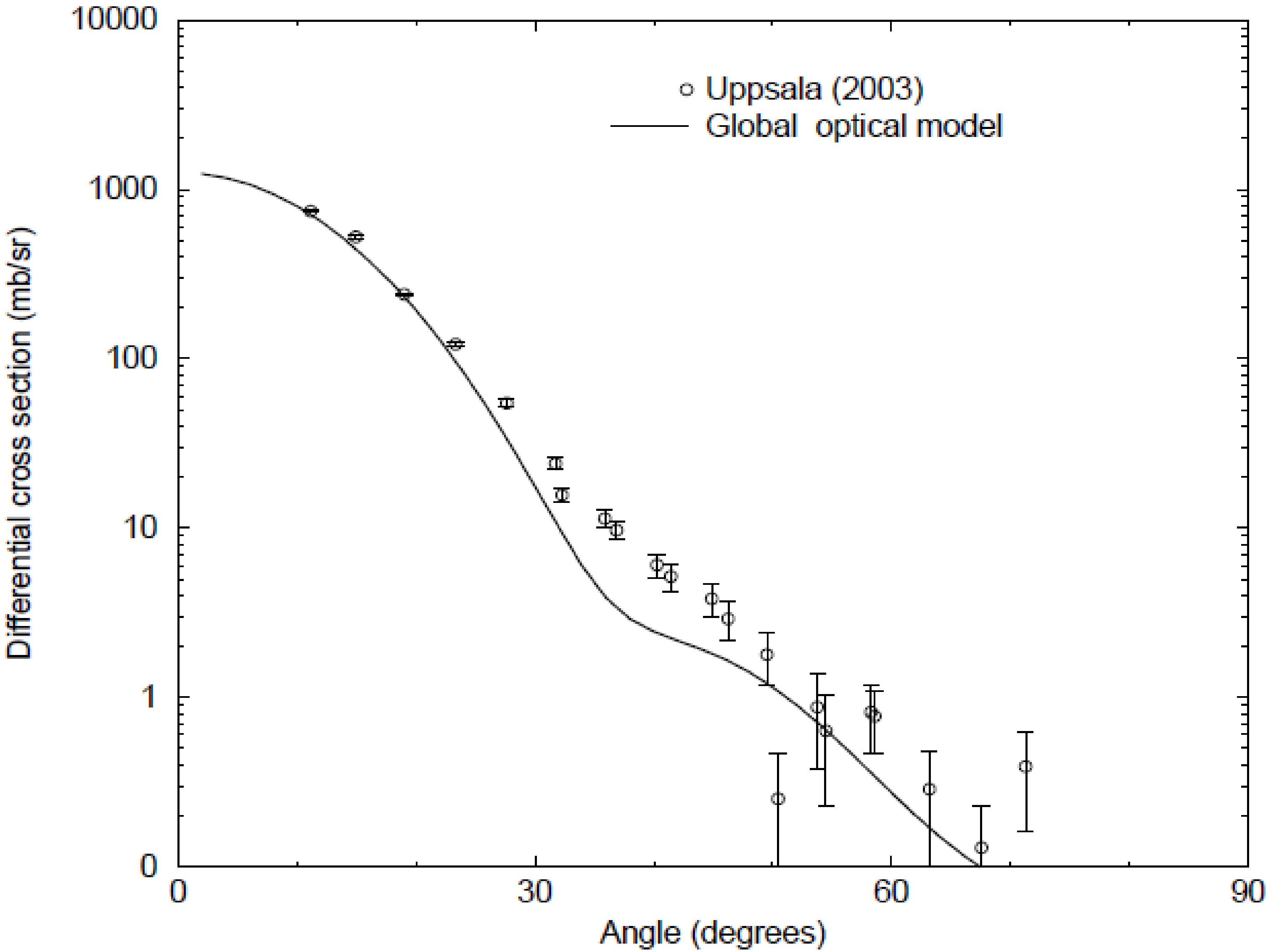


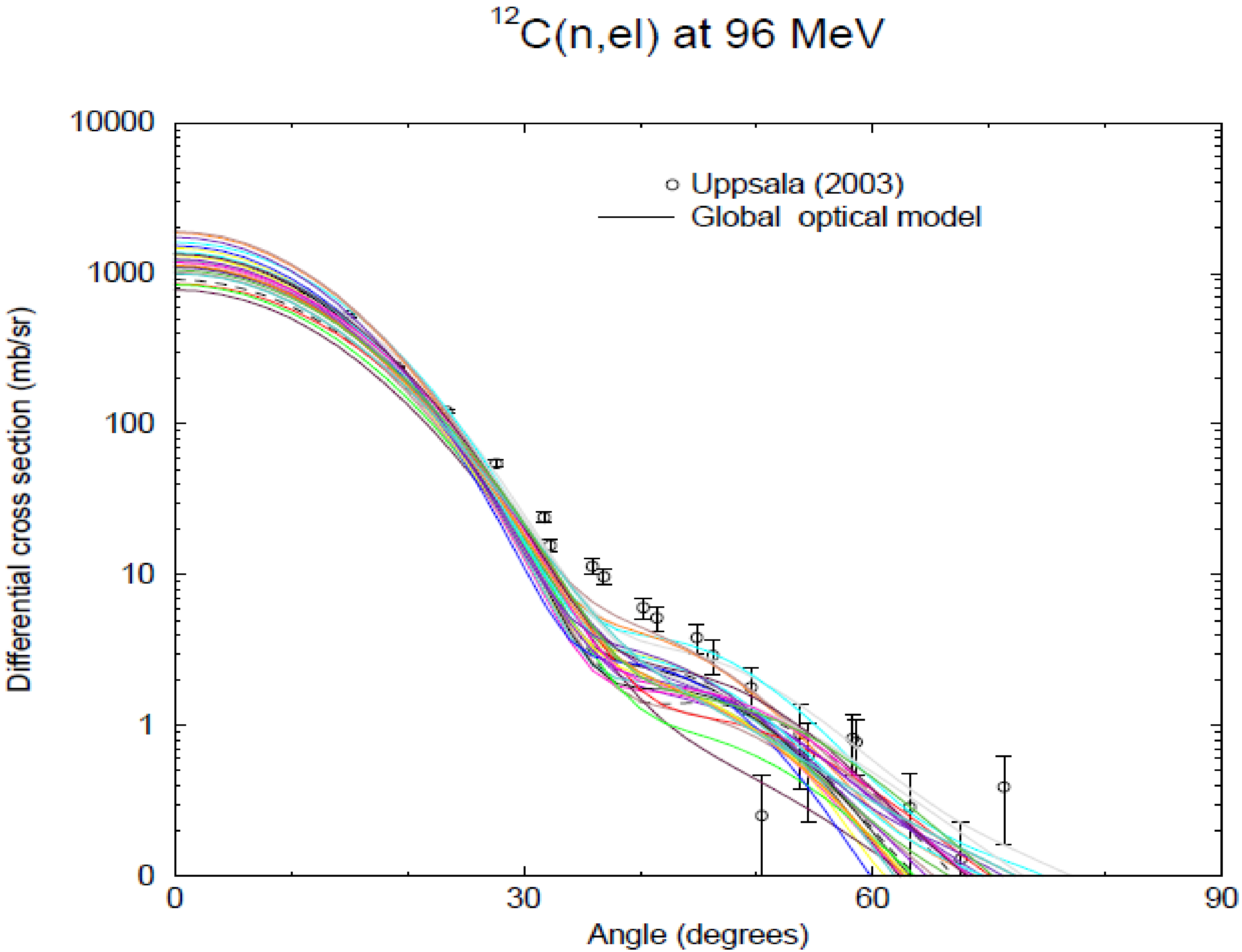
^{90}Zr (n,gamma)
(100 TALYS runs)
Cross section [mb]
E [MeV]
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-1}
10^0
10^1

$^{90}Zr(n,\gamma)$



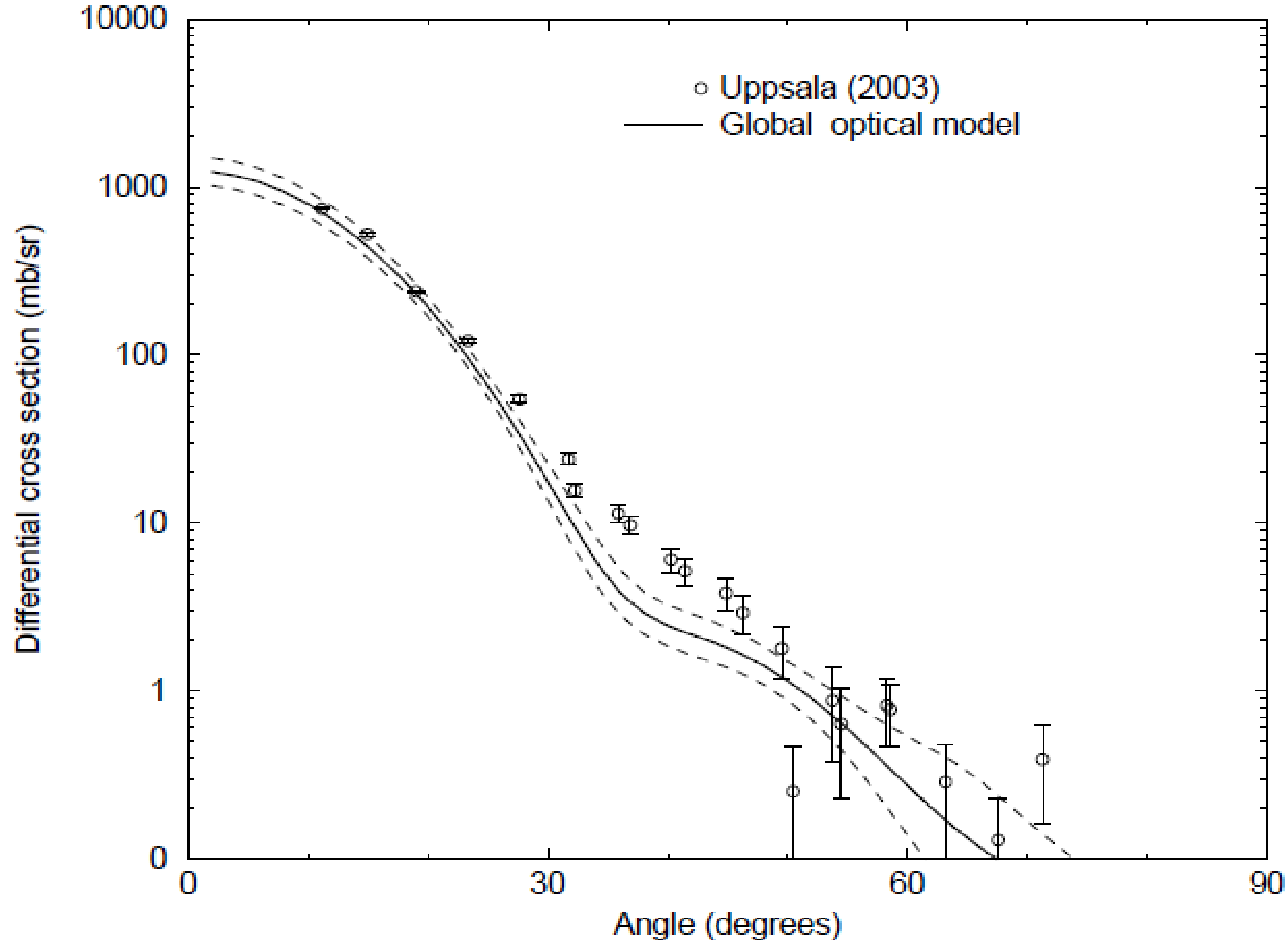
$^{12}C(n,el)$ at 96 MeV



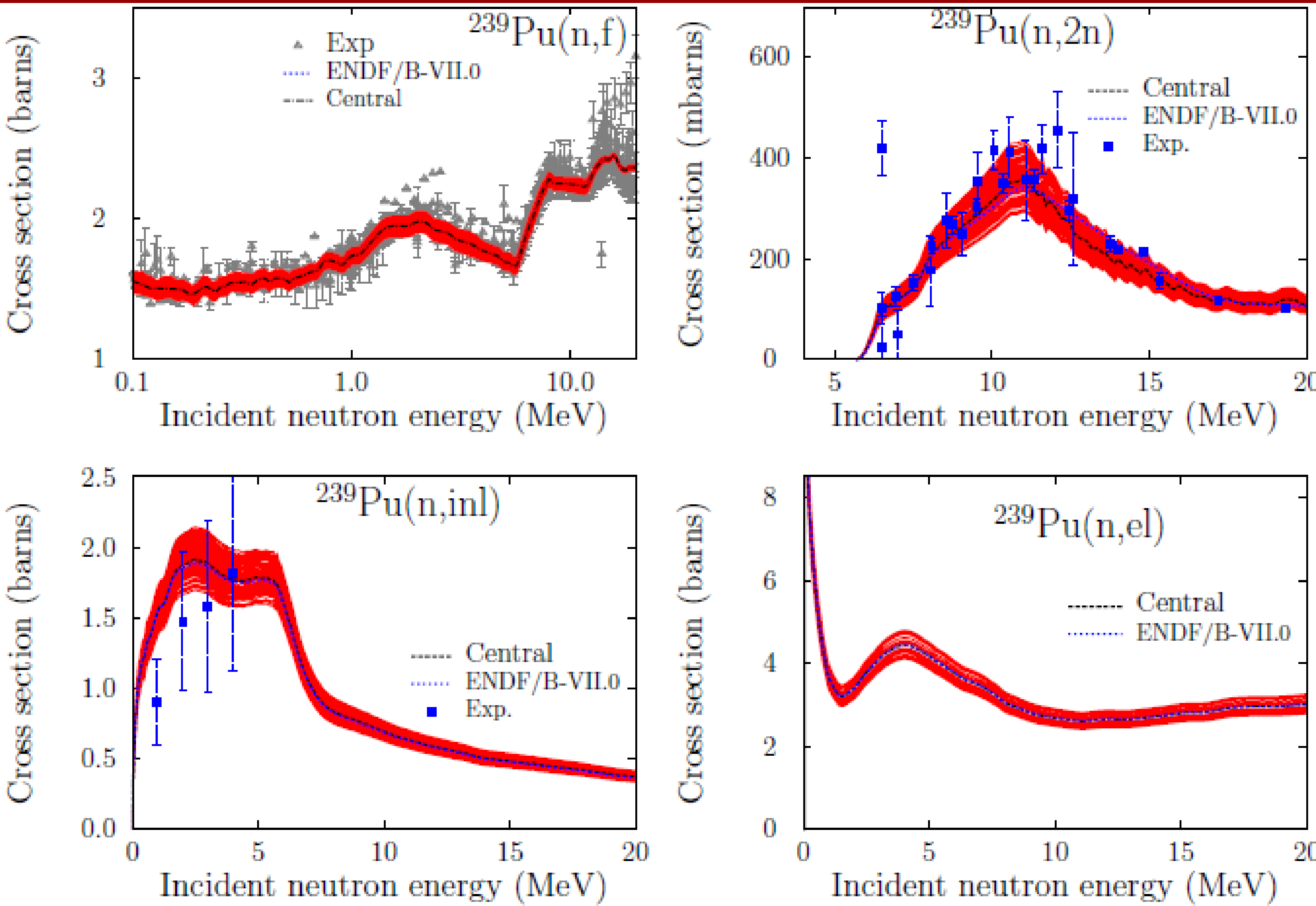


$^{12}C(n,el)$ at 96 MeV
Uppsala (2003)
Global optical model
10000
1000
100
10
1
0
0
30
60
90
Differential cross section (mb/sr)
Angle (degrees)

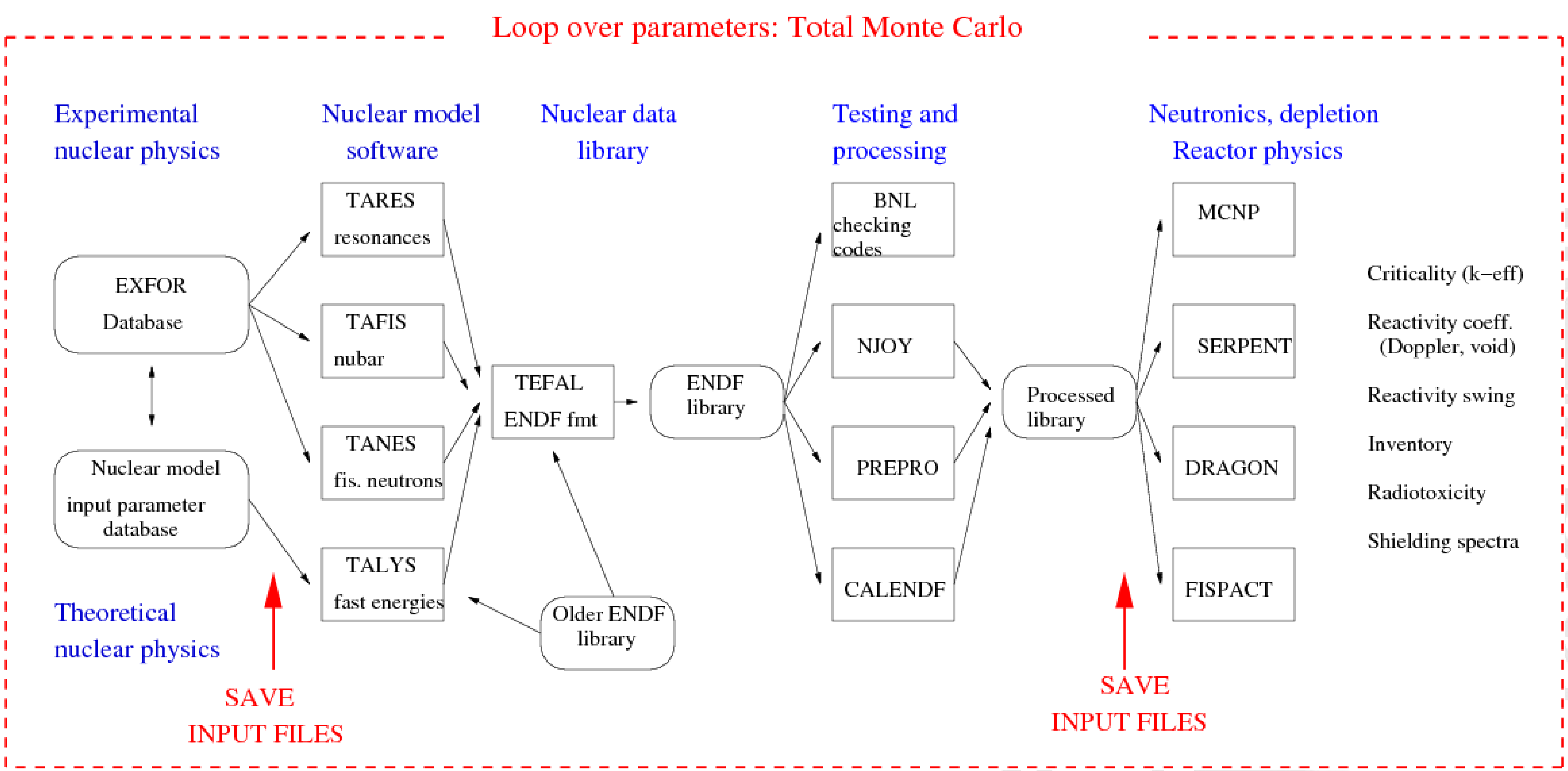
^{12}C(n,el) at 96 MeV



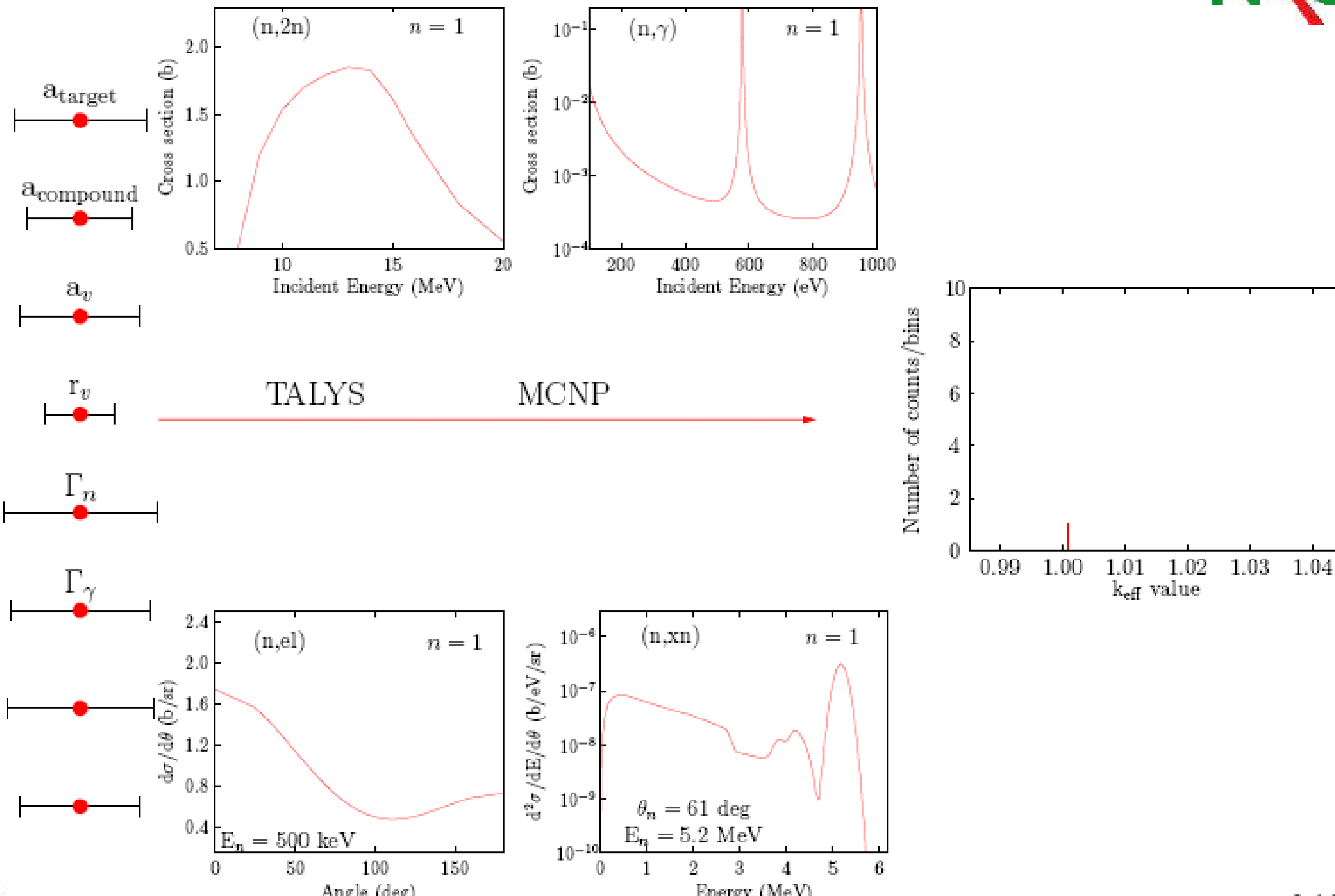
Random cross sections for ^{239}Pu



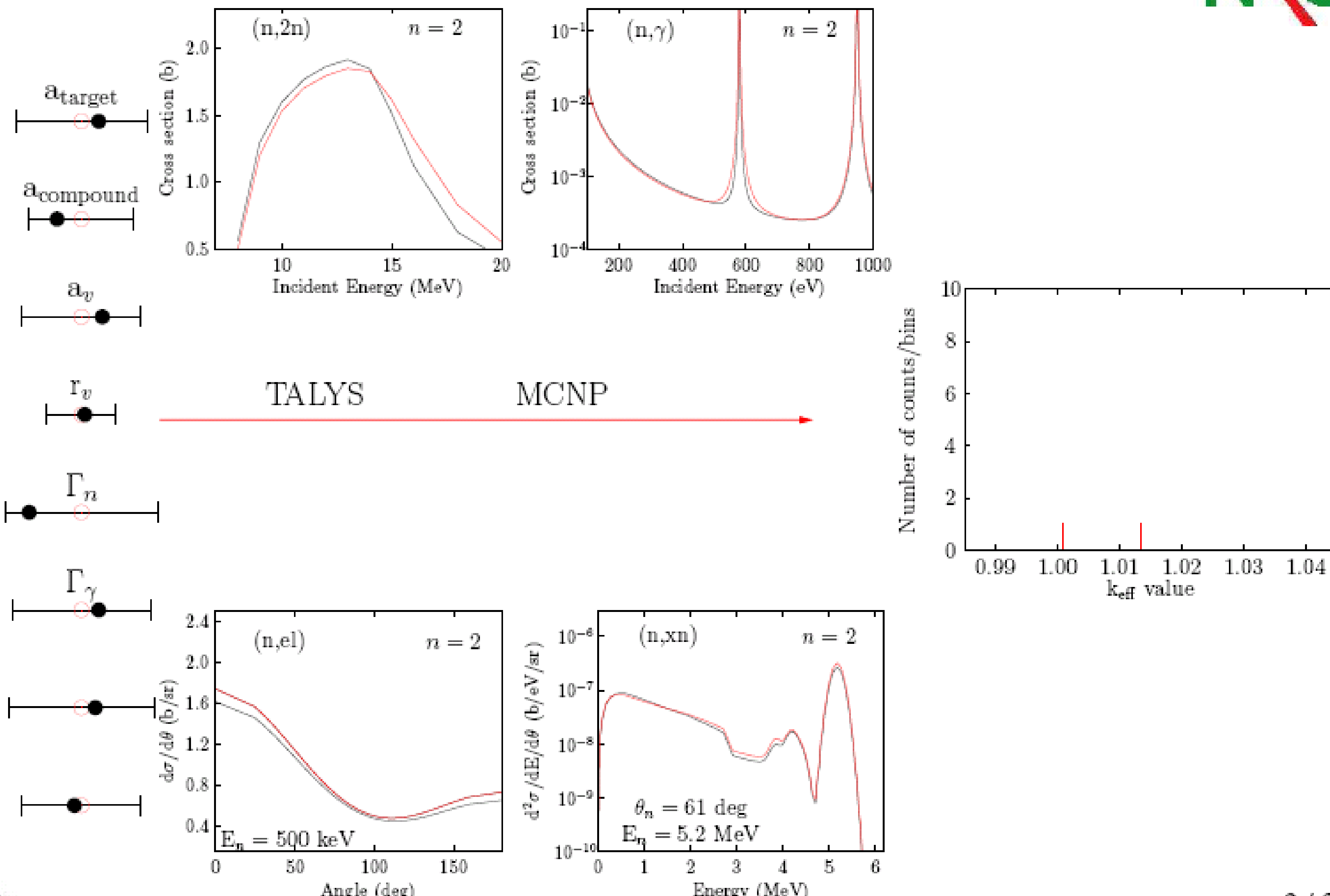
Total Monte Carlo



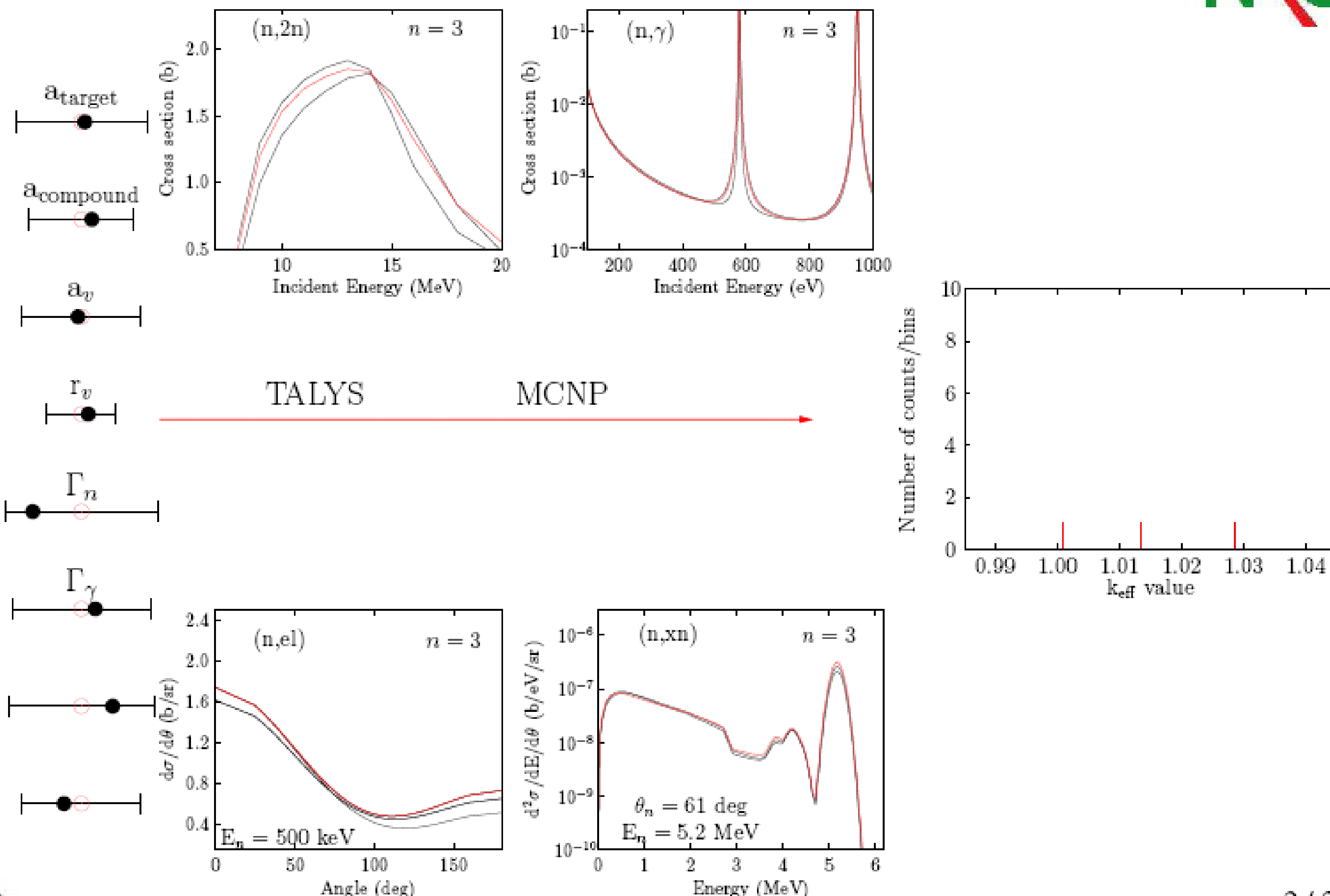
"1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb"



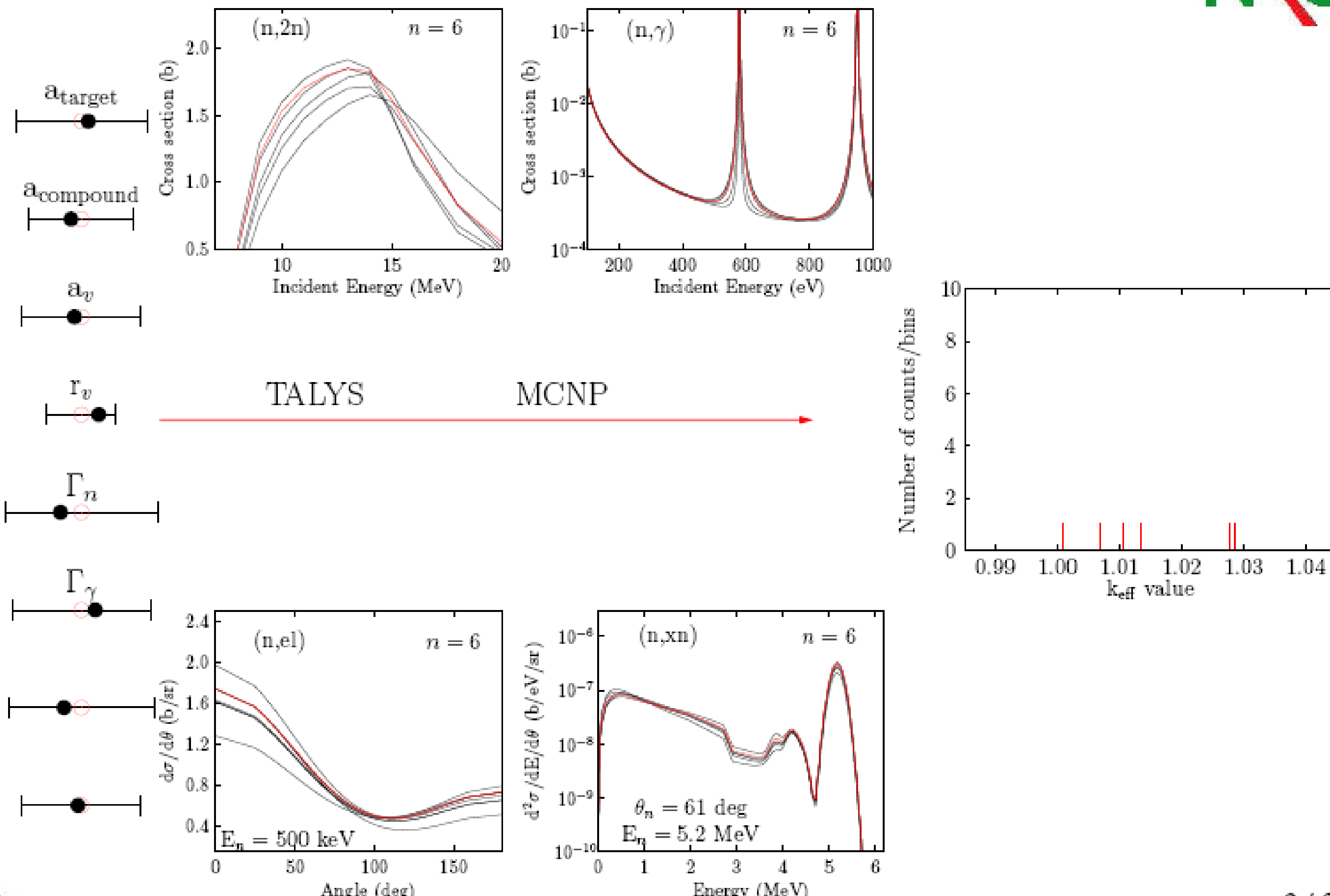
"1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb"



"1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb"



“1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb”



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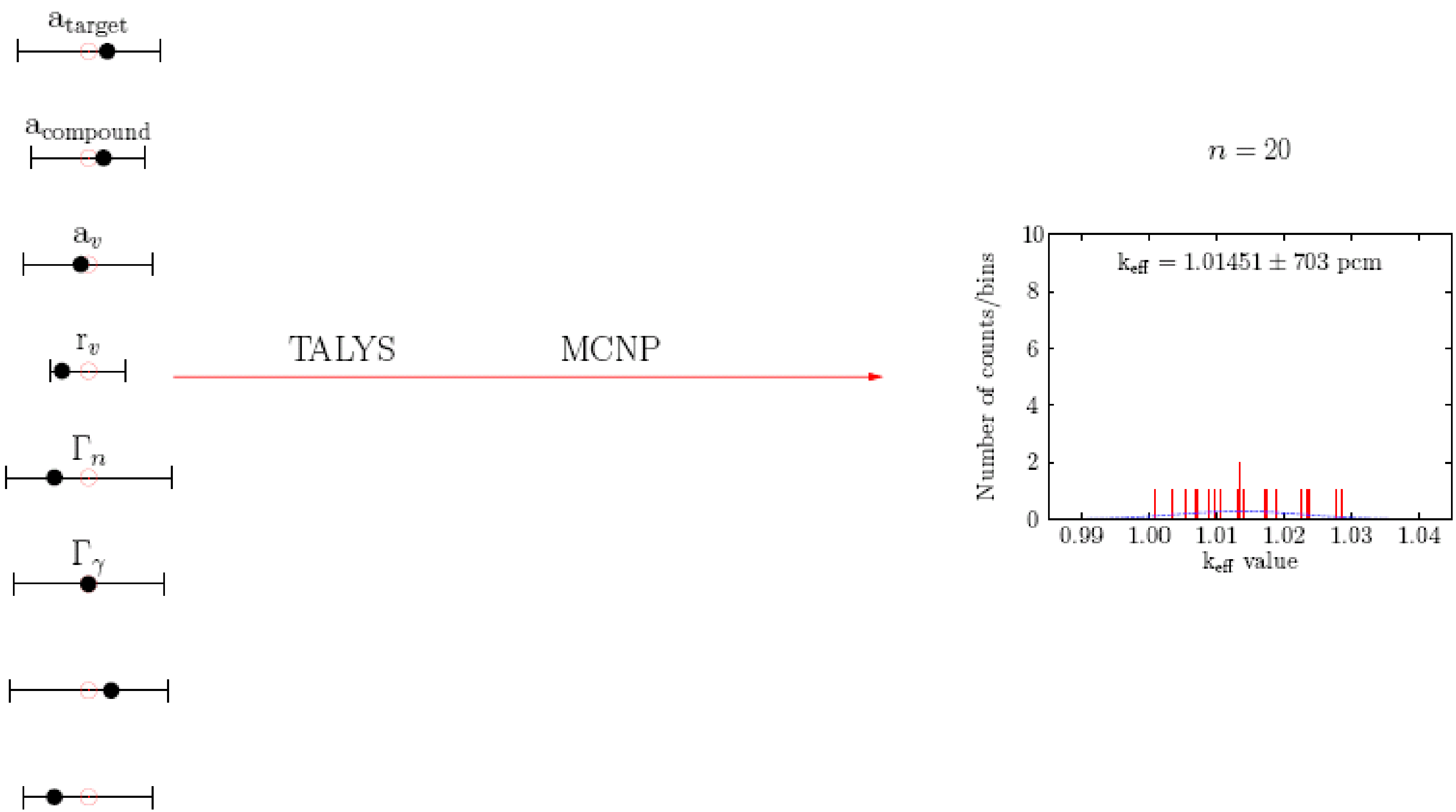

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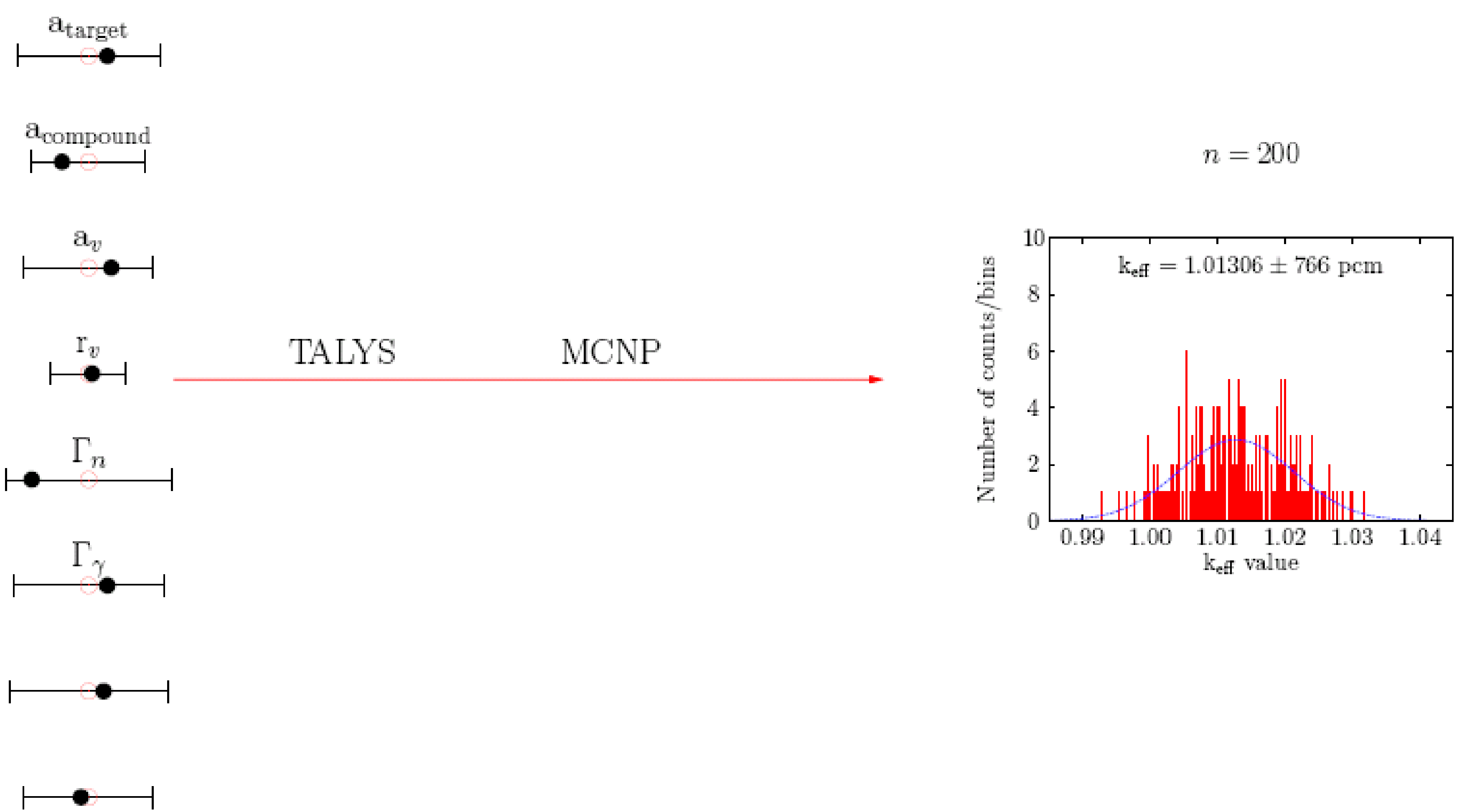

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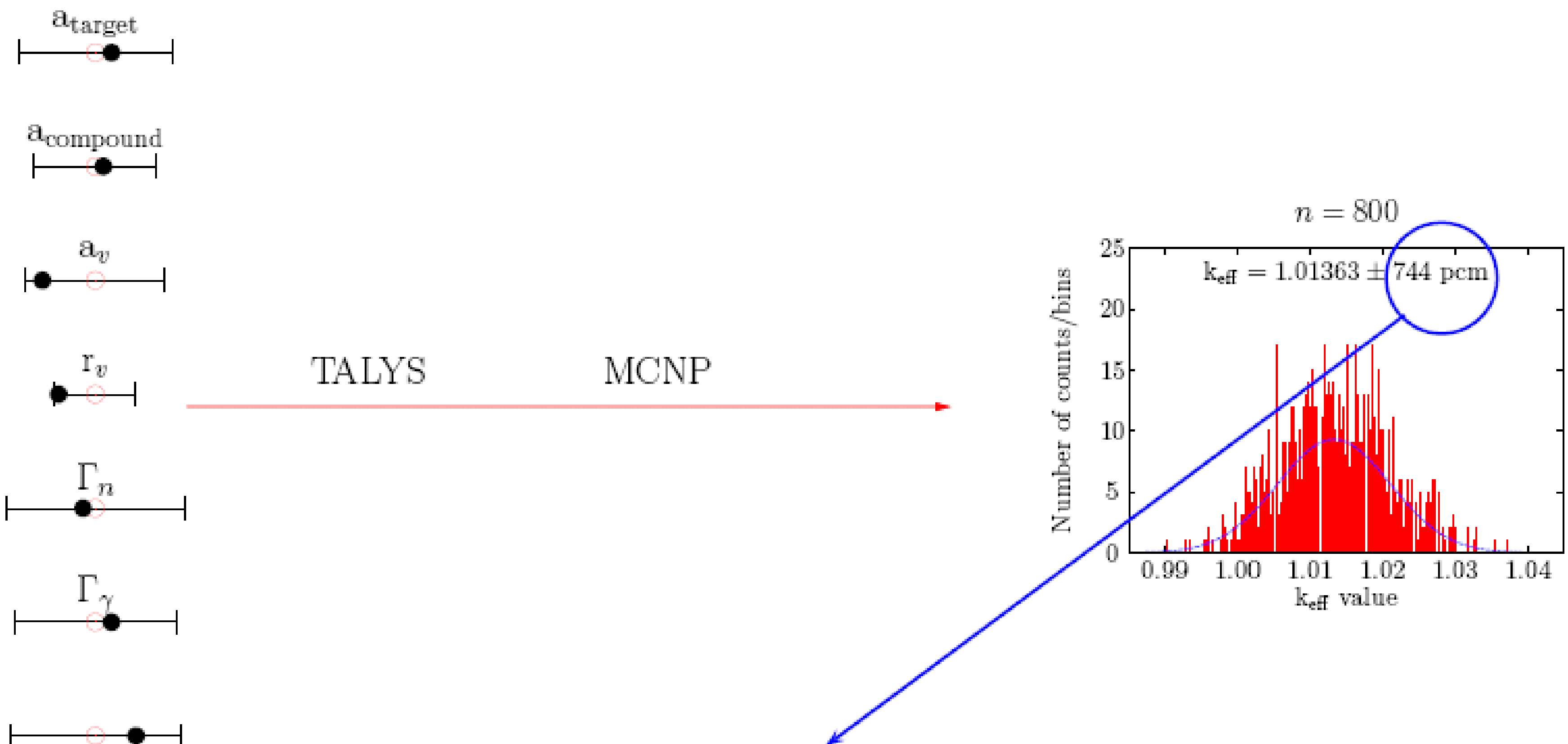

Statistical uncertainty $\simeq$ 68 pcm

$\Longrightarrow$ uncertainty due to nuclear data $\simeq$ 740 pcm

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Fusion: Optimized Cu-65 file: differential performance

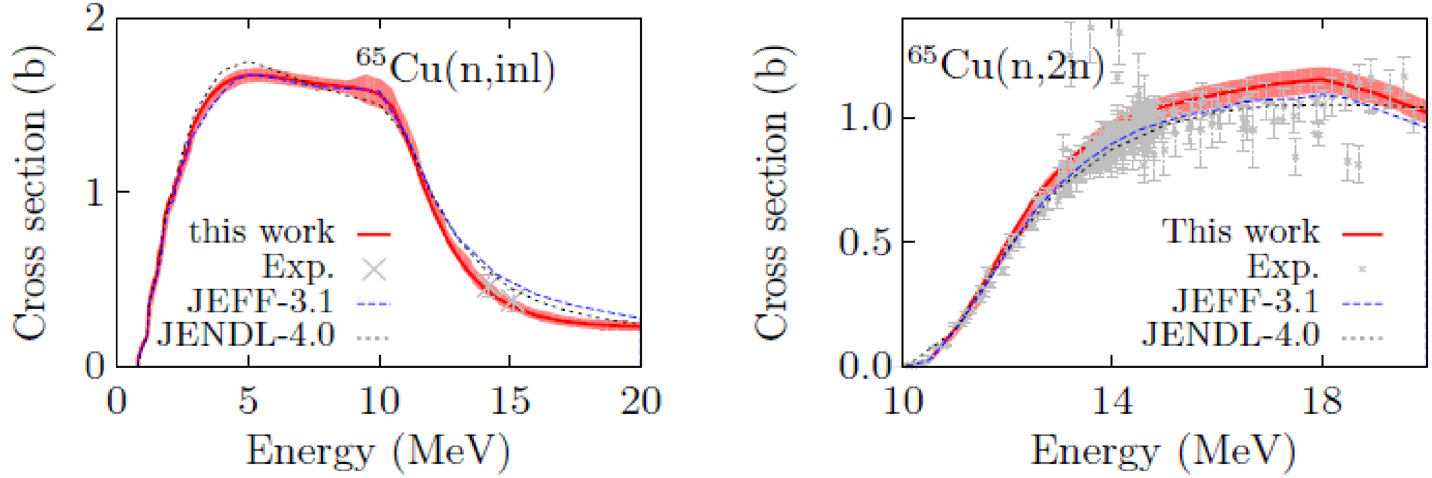
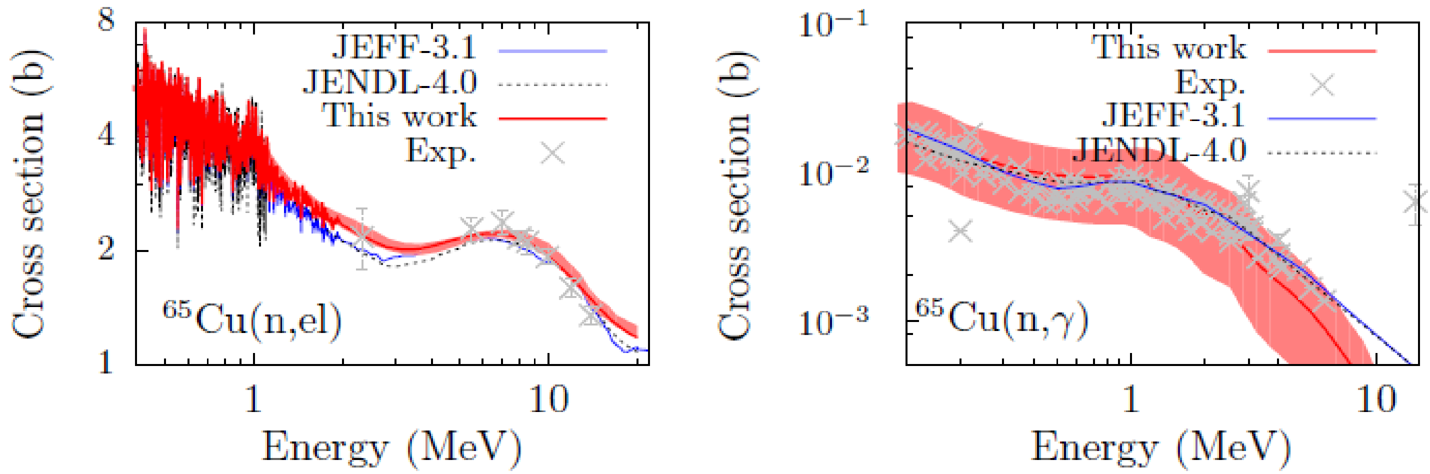
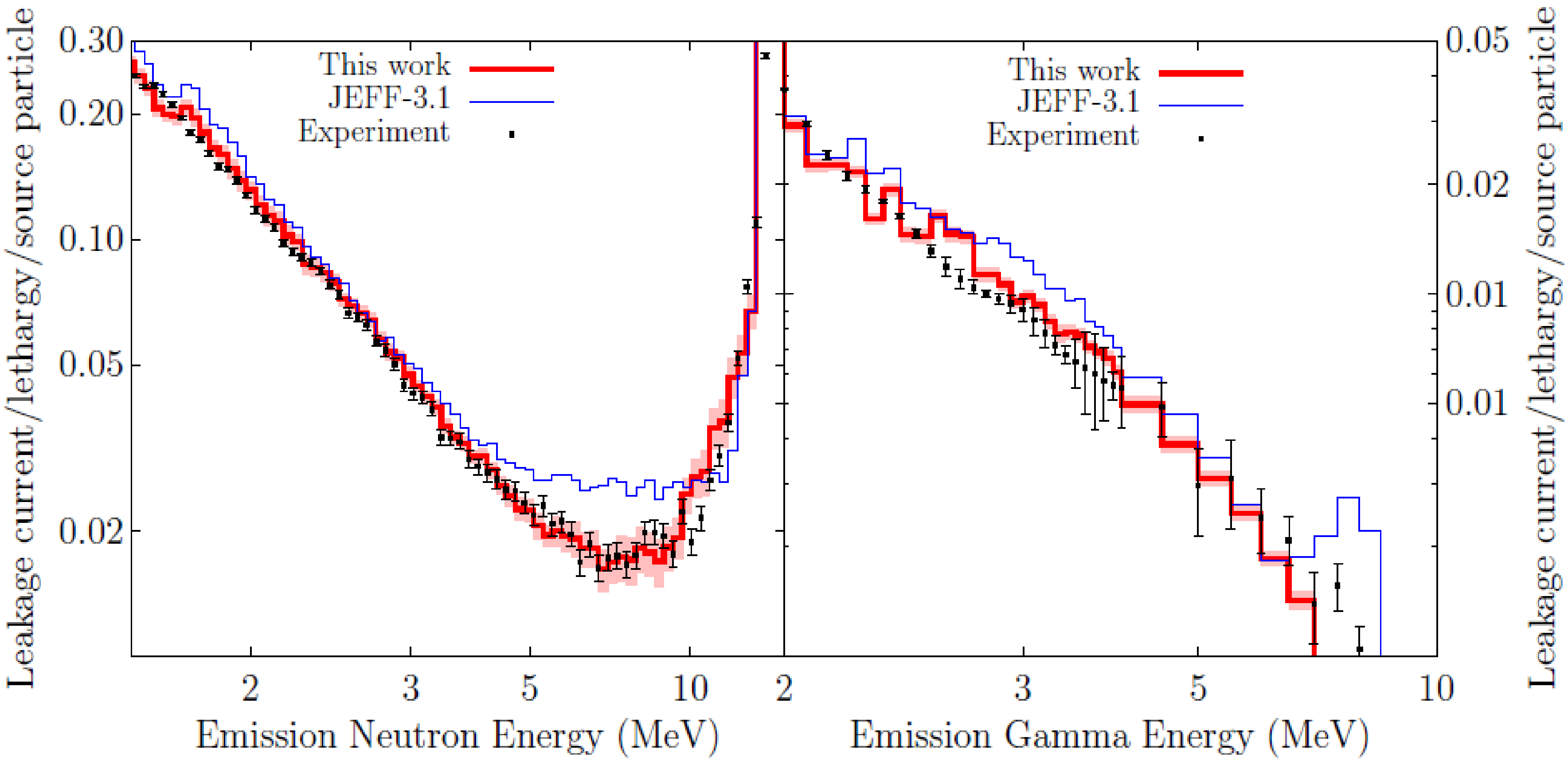


FIG. 12: Inelastic and (n,2n) cross sections for ^{65}Cu.



Fusion: Optimized Cu63,65 file vs Oktavian: integral performance

D. Rochman, A.J. Koning and S.C. van der Marck, ``Exact nuclear data uncertainty propagation for fusion design'', Fusion Engineering and Design 85, 669-682 (2010).



Summary

- TALYS (www.talys.eu) is
  - a user-friendly nuclear model code for reactions involving all light particles up to 200 MeV,
  - used, and validated, by a worldwide community,
  - competitive at all energies
  - Used to analyze nuclear reaction experiments
  - Capable of producing complete nuclear reaction data sets of reasonable to good quality for all kinds of applications