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Use of TALYS for Model Estimation of Evaluated Data Uncertainties

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Uncertainties in nuclear data

- Since no stage in nuclear science is perfectly under control, all scientific results should come with uncertainties (or more generally, covariance data).
- All nuclear experiments and nuclear model codes have uncertainties. Nuclear data evaluation should consider
  - probability distributions (exact), or
  - covariances (most popular from users side), or
  - variances (for the older codes),
- Use a combination of experimental and theoretical uncertainties.

Fast reactors: Target accuracies from industry and research (CEA + AREVA table)

Table 1. Fast Reactor and ADMAB Target Accuracies (1σ)

Multiplication factor (BOL)	300 pcm
Power peak (BOL)	2%
Burnup reactivity swing	300 pcm
Reactivity coefficients (Coolant void and Doppler - BOL)	7%
Major nuclide density at end of irradiation cycle	2%
Other nuclide density at end of irradiation cycle	10%

Required nuclear data uncertainties (Salvatores et al, SG 26)

Table 1. Summary Target Accuracies for Fast Reactors

		Energy Range	Current Accuracy (%)	Target Accuracy (%)
U238	σ_{inel}	6.07 ÷ 0.498 MeV	10 ÷ 20	2 ÷ 3
	σ_{capt}	24.8 ÷ 2.04 keV	3 ÷ 9	1.5 ÷ 2
Pu241	σ_{fiss}	1.35MeV ÷ 454 eV	8 ÷ 20	2 ÷ 3 (SFR,GFR,LFR) 5 ÷ 8 (ABTR,EFR)
Pu239	σ_{capt}	498 ÷ 2.04 keV	7 ÷ 15	4 ÷ 7
Pu240	σ_{fiss}	1.35 ÷ 0.498 MeV	6	1.5 ÷ 2
	ν	1.35 ÷ 0.498 MeV	4	1 ÷ 3
Pu242	σ_{fiss}	2.23 ÷ 0.498 MeV	19 ÷ 21	3 ÷ 5
Pu238	σ_{fiss}	1.35 ÷ 0.183 MeV	17	3 ÷ 5
Am242m	σ_{fiss}	1.35MeV ÷ 67.4keV	17	3 ÷ 4
Am241	σ_{fiss}	6.07 ÷ 2.23 MeV	12	3
Cm244	σ_{fiss}	1.35 ÷ 0.498 MeV	50	5
Cm245	σ_{fiss}	183 ÷ 67.4 keV	47	7
Fe56	σ_{inel}	2.23 ÷ 0.498 MeV	16 ÷ 25	3 ÷ 6
Na23	σ_{inel}	1.35 ÷ 0.498 MeV	28	4 ÷ 10
Pb206	σ_{inel}	2.23 ÷ 1.35 MeV	14	3
Pb207	σ_{inel}	1.35 ÷ 0.498 MeV	11	3
Si28	σ_{inel}	6.07 ÷ 1.35 MeV	14 ÷ 50	3 ÷ 6
	σ_{capt}	19.6 ÷ 6.07 MeV	53	6

Uncertainties in nuclear data

Experimentalists:

- are well educated: give uncertainties with their results.
- But, not seldom:
  - wrong systematical errors (usually underestimated), or,
  - no systematical errors given at all
- Difficult to establish good covariance data file, especially for correlation between different reaction channels (usually obtained from different labs).

Uncertainties in nuclear data

Theoreticians:

- Good behaviour: some don't stop until all reaction channels are completely predicted.
- 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

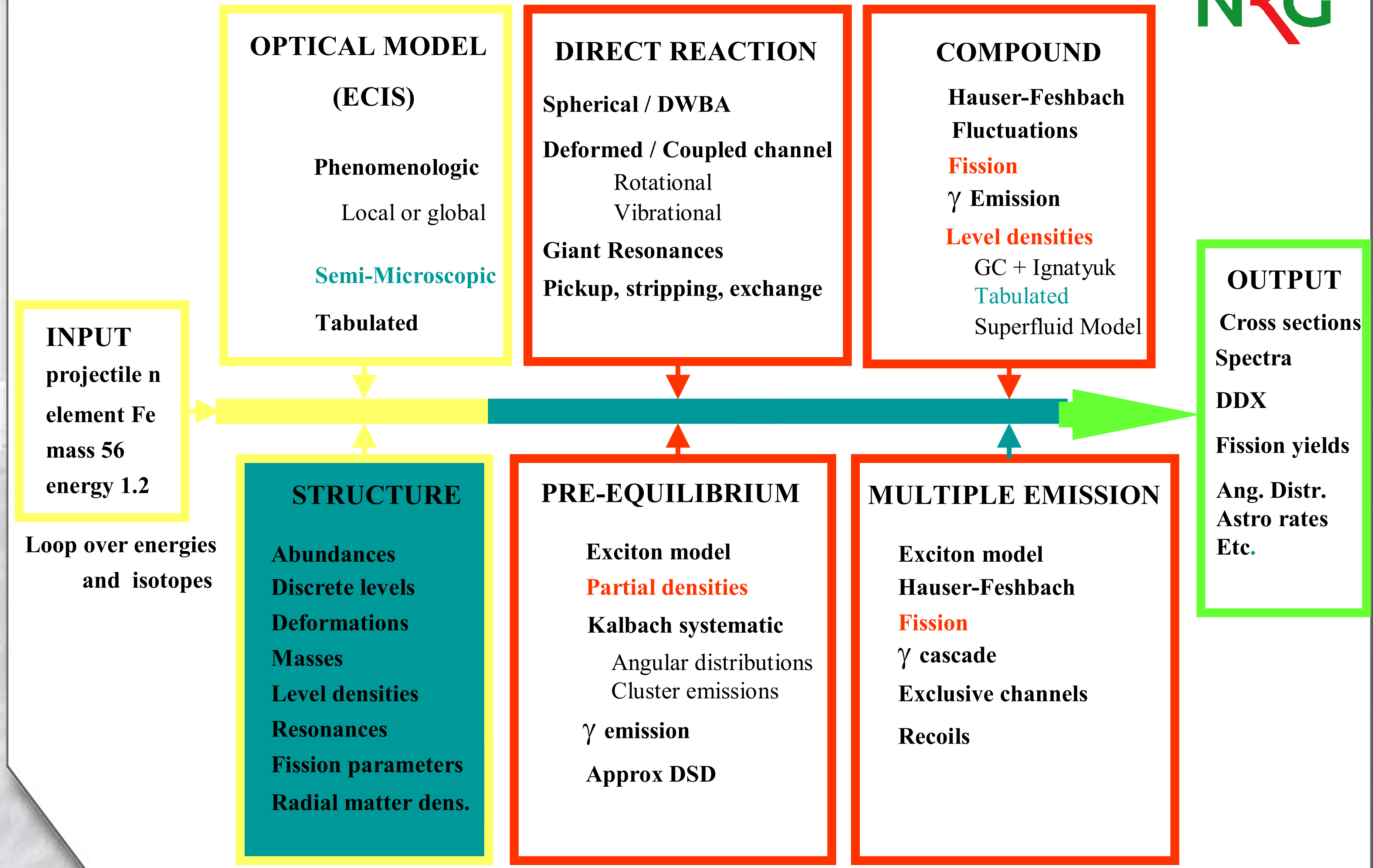
No excuse possible:

- 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, fission yields, etc.?

Uncertainties with nuclear models

- 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).

TALYS code scheme



TALYS-1.2

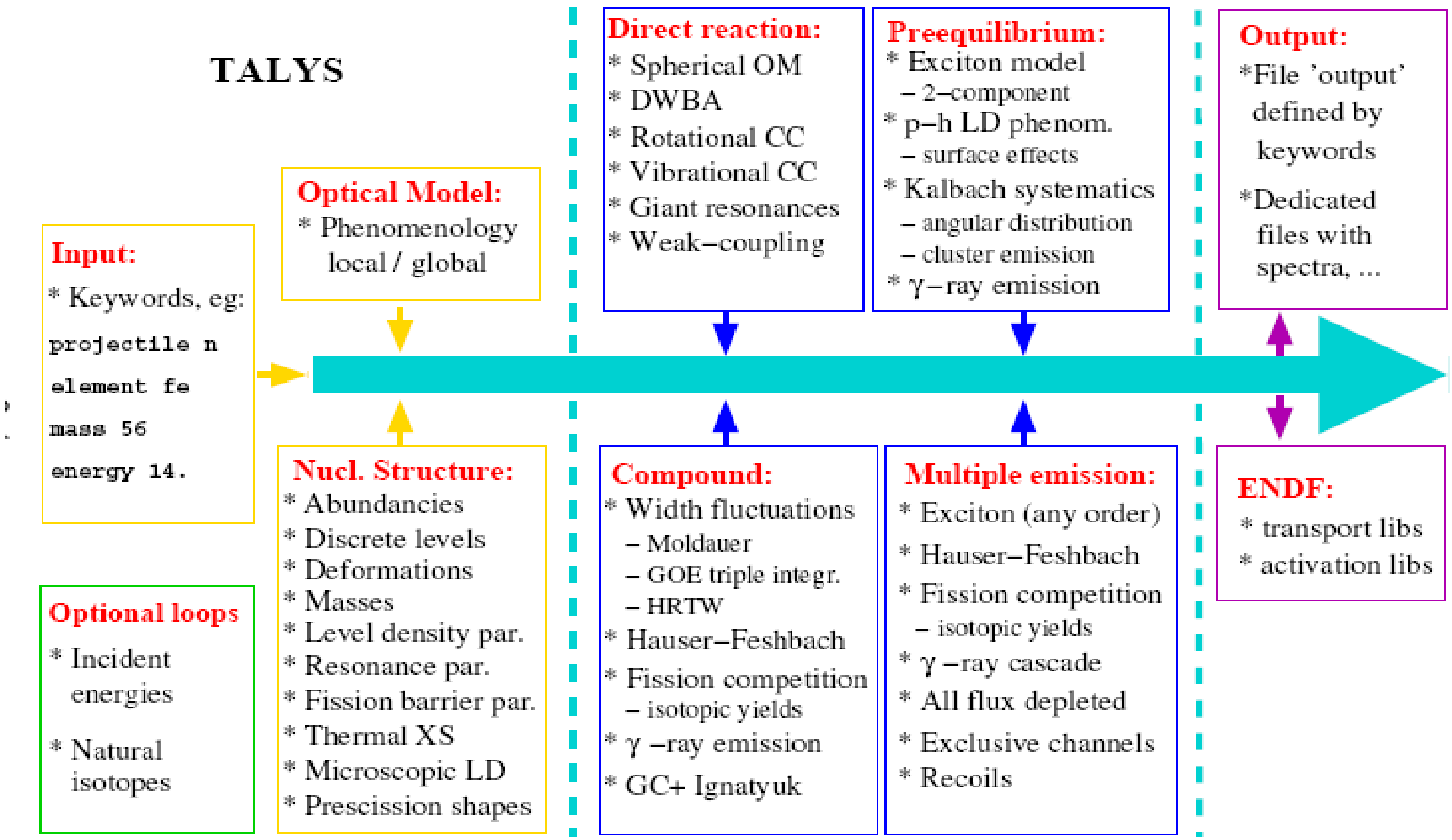
- Released December 21, 2009, see www.talys.eu
- Use of TALYS increasing
  - Estimated 400-500 users, 160-200 publications
- Some recent improvements for TALYS-1.2:
  - Better fission + level density model (CEA Bruyeres-le-Chatel)
  - The option to easily/safely store the best input parameter set per nucleus (“best y”)
  - More flexibility for covariance development and adjustment to experimental data
- TALYS can be used for
  - In-depth nuclide/reaction analyses
  - Global multi-nuclide calculations
  - These two are now being merged

Uncertainties with nuclear models

- Nuclear model parameter vector $\mathbf{p}$: 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.

At the end, replace σ_0 by the **average** cross section

TALYS uses many parameters!!!



Sample input file for TALYS

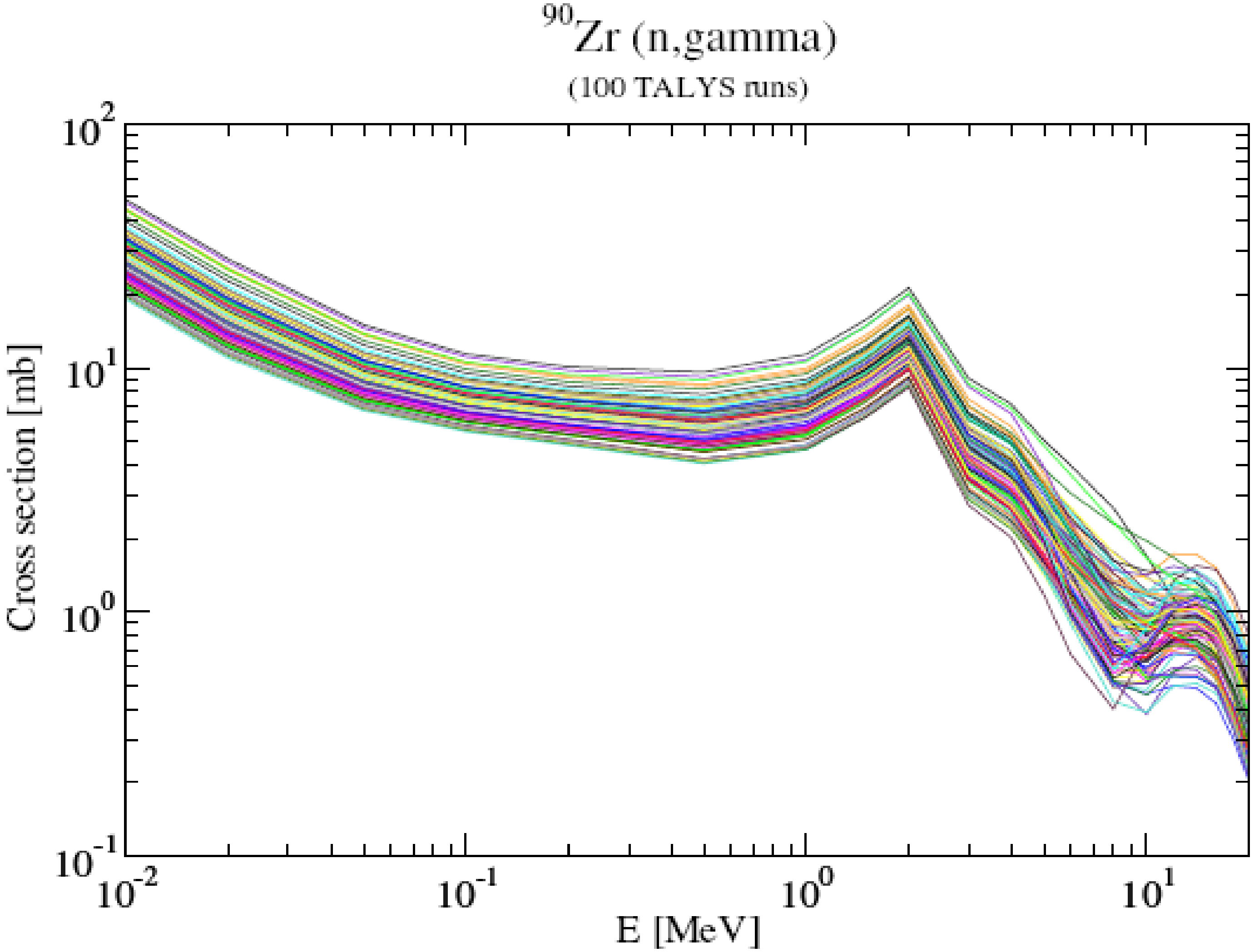
Input file 0 (Central values)

```
projectile n
element fe
mass 56
energy energies
#
#General parameters
#
M2constant 1.
#
# Parameters for  57Fe
#
a          26  57   6.77226
gammald    26  57   0.11927
gamgam     26  57   0.92000
sgr        26  57  83.976 E1
..........................
```

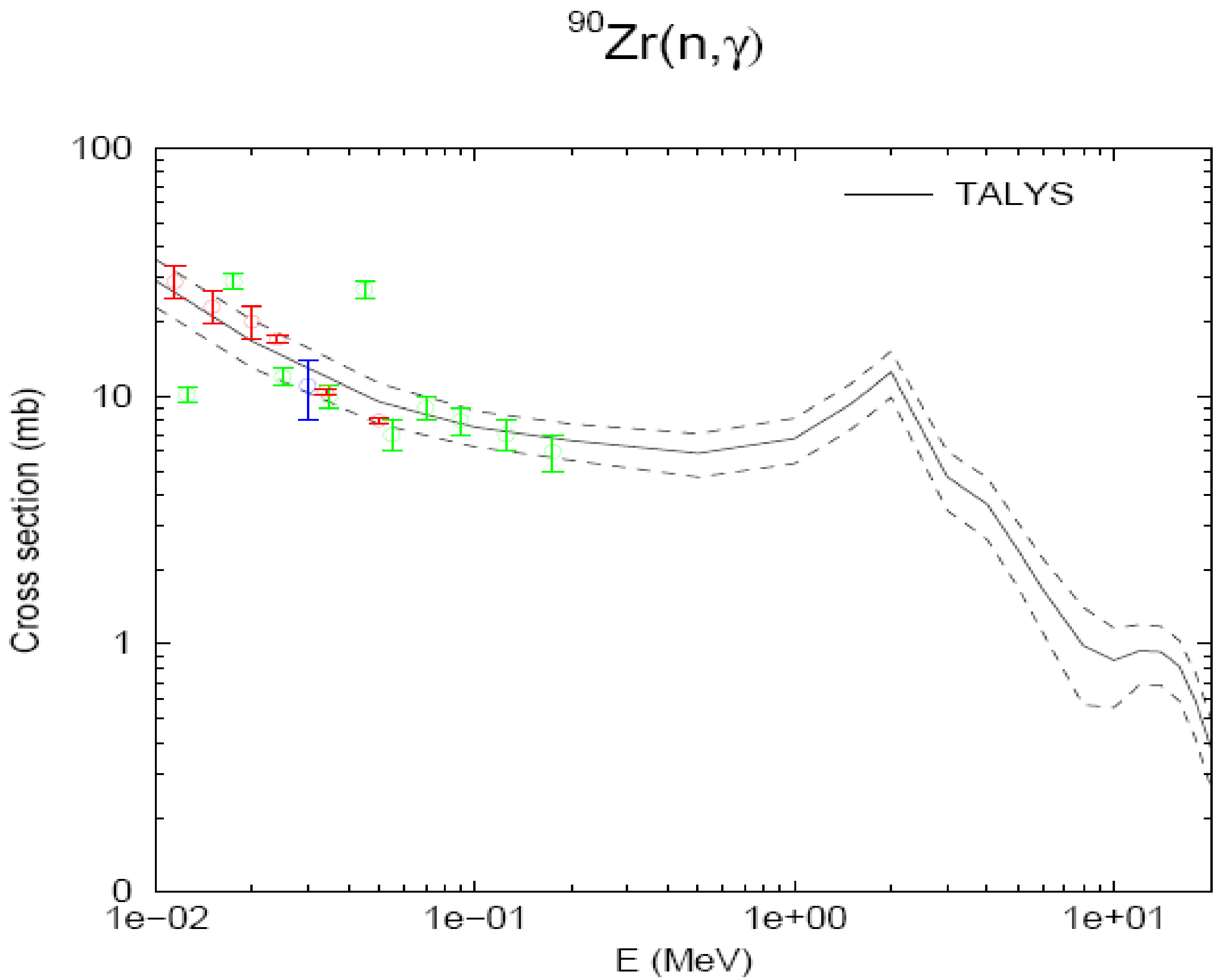
Input file 1

```
projectile n
element fe
mass 56
energy energies
#
#General parameters
#
M2constant 1.19515
#
# Parameters for  57Fe
#
a          26  57   6.29336
gammald    26  57   0.17733
gamgam     26  57   0.69751
sgr        26  57 102.600 E1
..........................
```

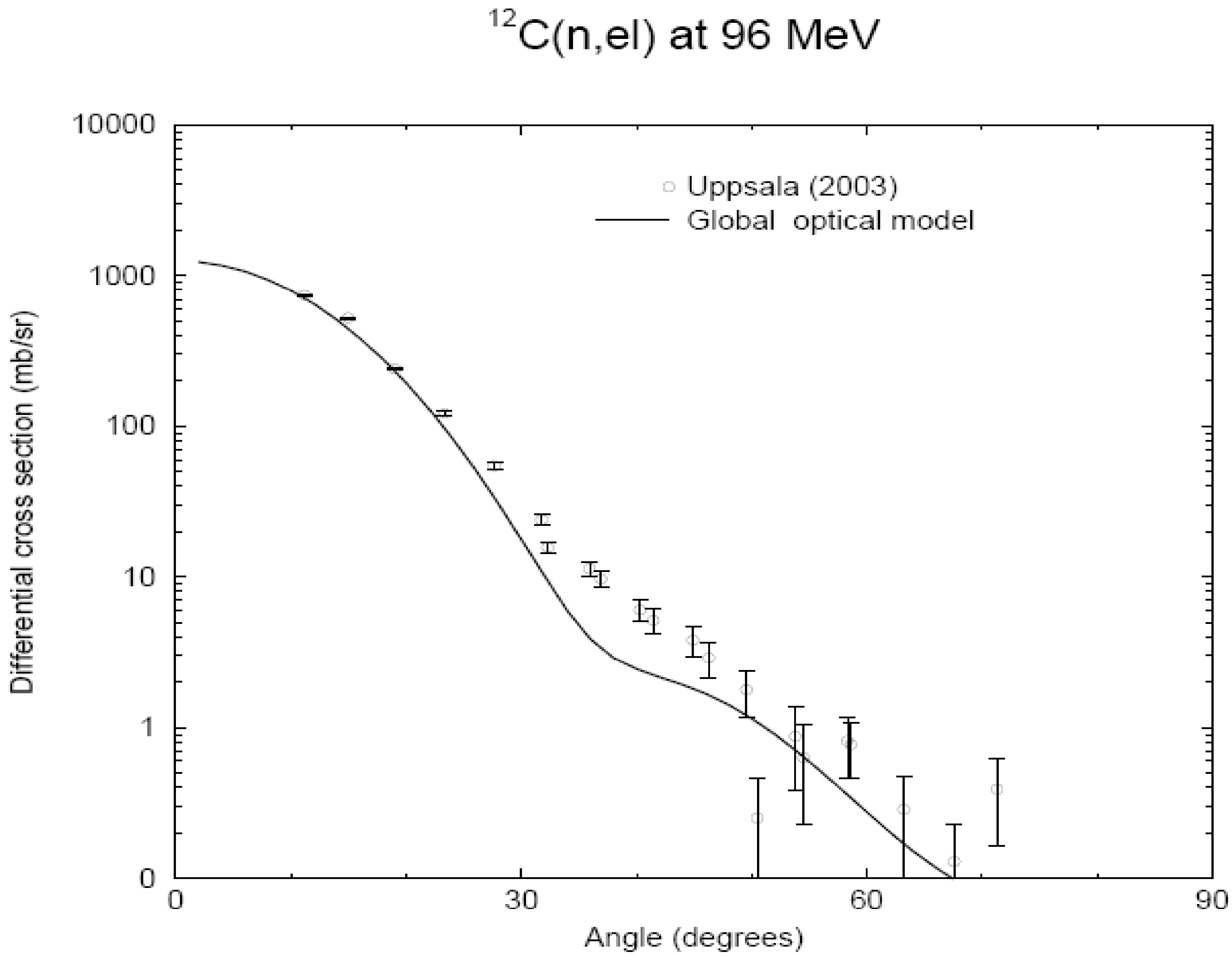
Random nuclear model calculations



Average: TALYS + uncertainty

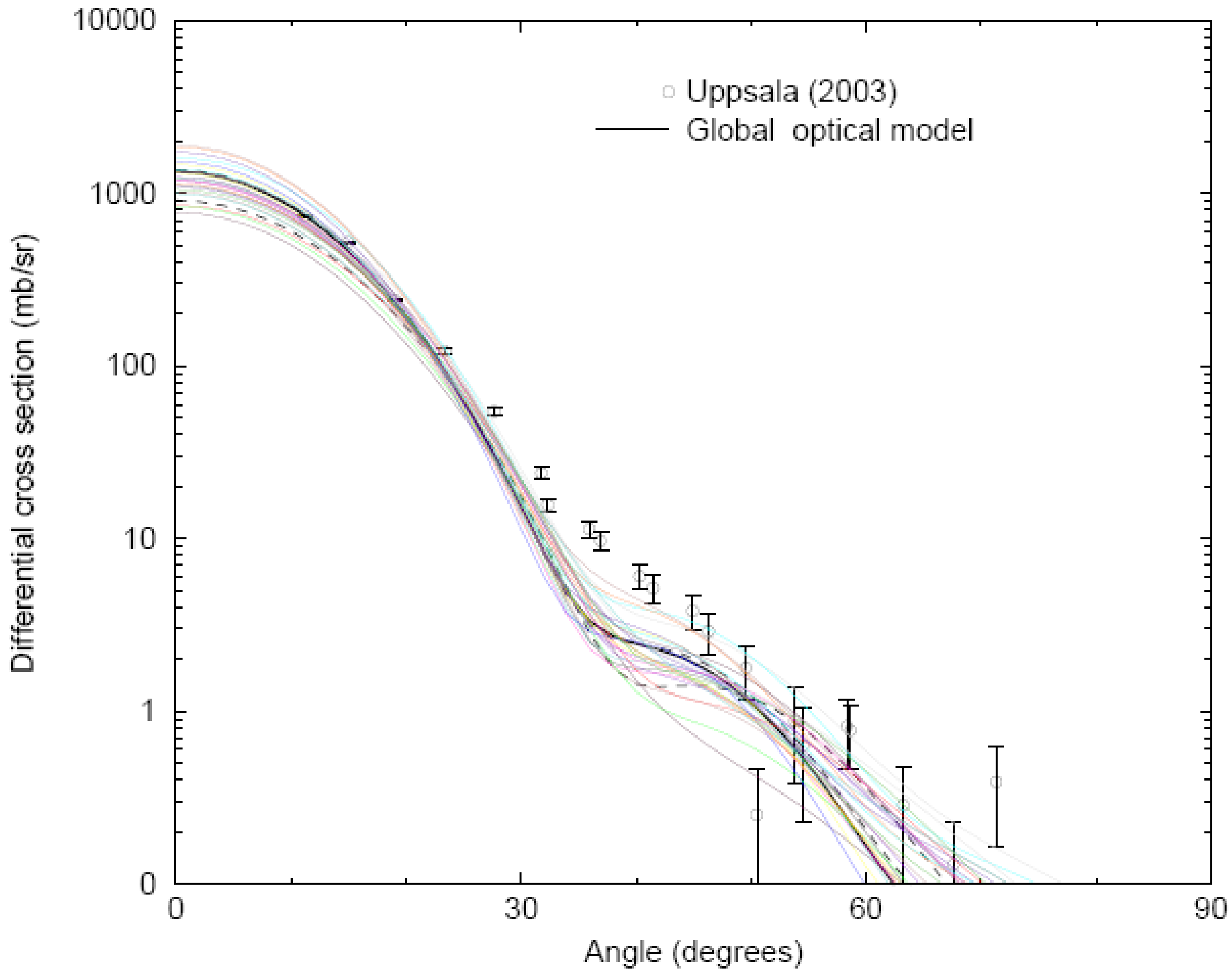


OMP uncertainties: high energies

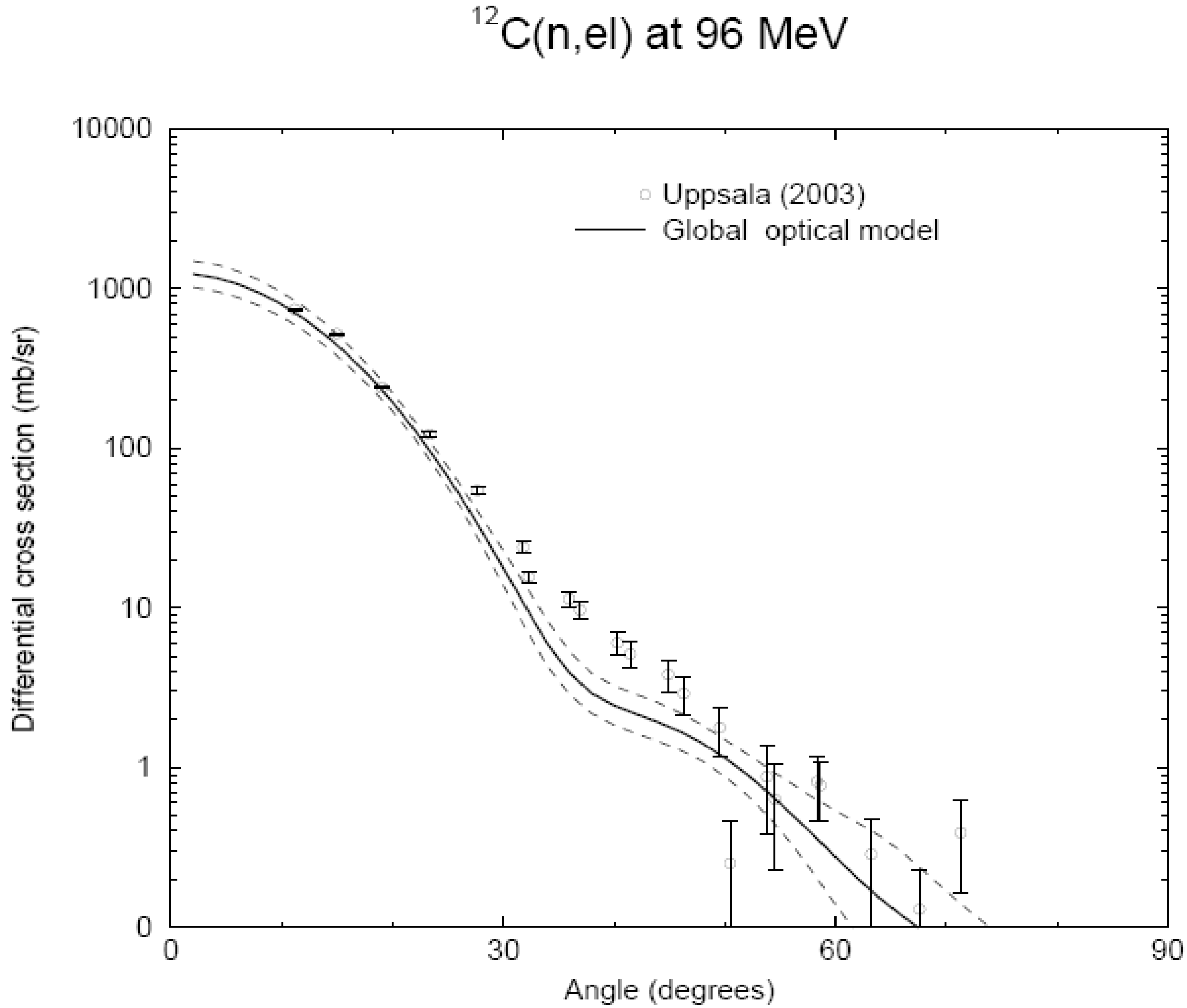


OMP uncertainties: high energies

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



OMP uncertainties: high energies



Example: parameter uncertainties for Pb

$$V_V(E) = v_1[1 - v_2(E - E_f) + v_3(E - E_f)^2 - v_4(E - E_f)^3],$$

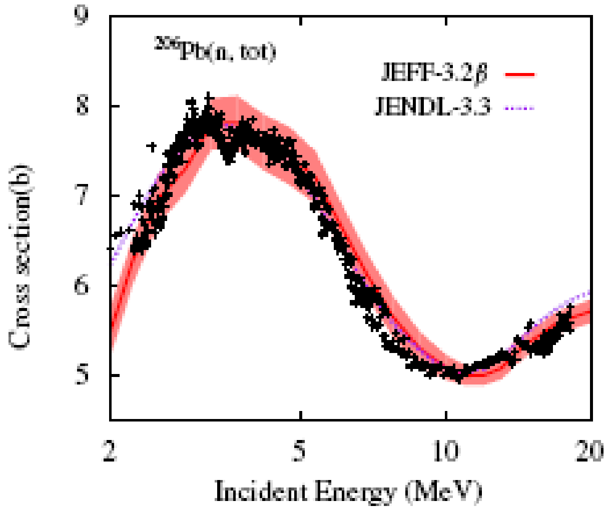
$$W_V(E) = w_1 \frac{(E - E_f)^2}{(E - E_f)^2 + (w_2)^2},$$

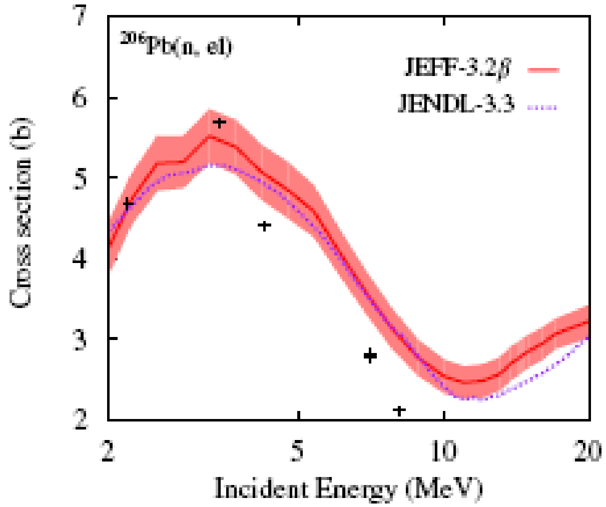
$$W_D(E) = d_1 \frac{(E - E_f)^2}{(E - E_f)^2 + (d_3)^2} \exp[-d_2(E - E_f)],$$

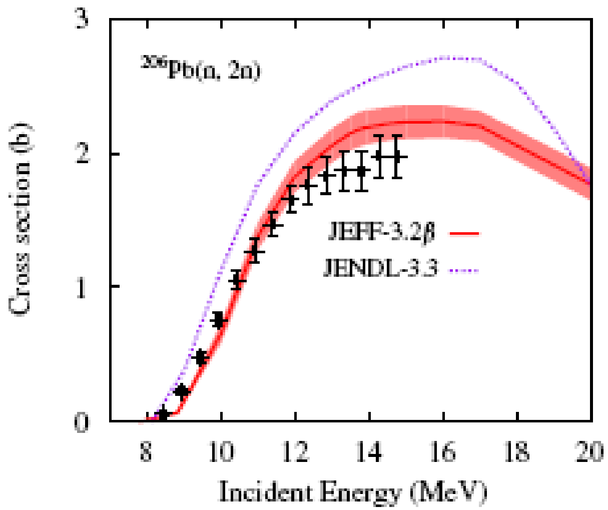
Koning-Delaroche OMP

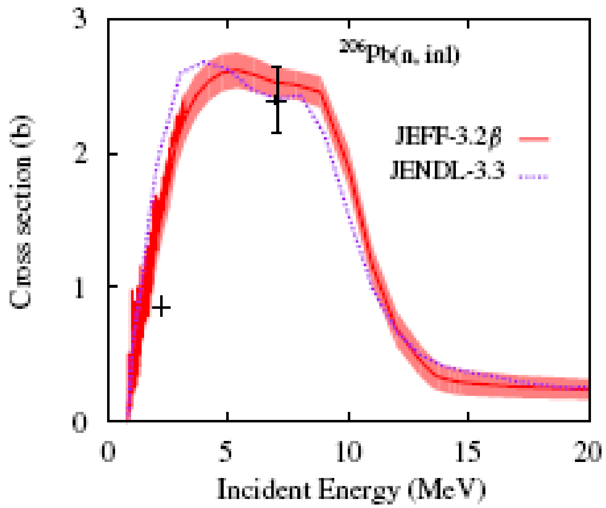
Parameter	Uncertainty (%)	Parameter	Uncertainty (%)
r_V	1.5	d_1^n	9.4
a_V	2.0	d_2^n	10
v_1^n	1.9	d_3^n	9.4
v_2^n	3.0	r_{SO}	9.7
v_3^n	3.1	a_{SO}	10
v_4^n	5.0	v_{so1}^n	5.0
w_1^n	9.7	v_{so2}^n	10
w_2^n	10	w_{so1}^n	20
r_D	3.5	w_{so2}^n	20
a_D	4.0	$M2$	21

Resulting uncertainties for Pb

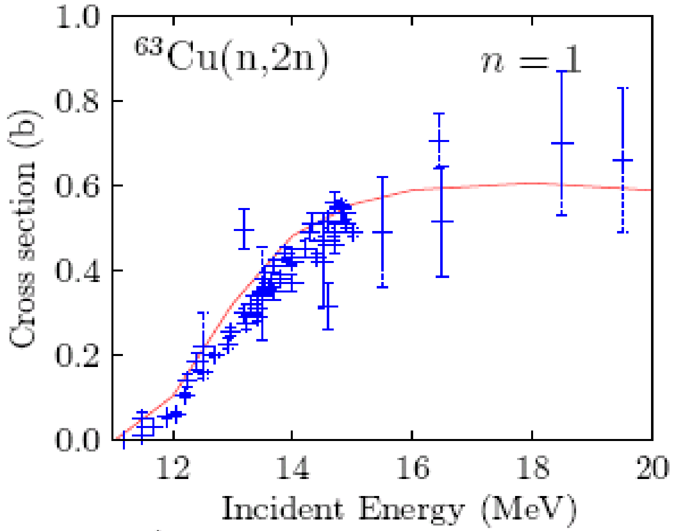


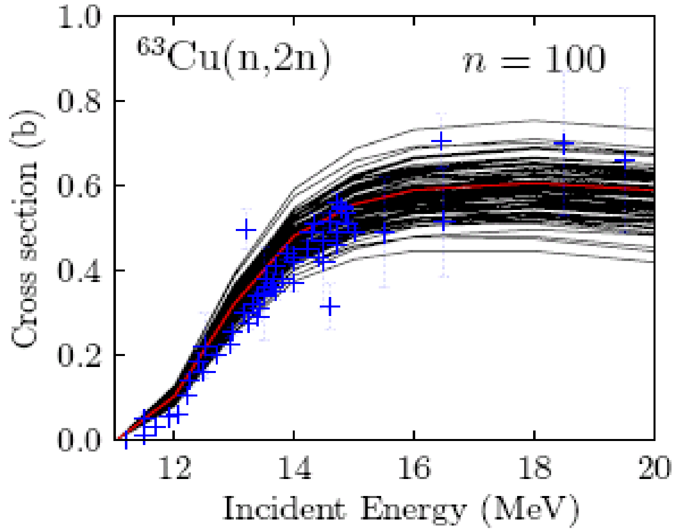


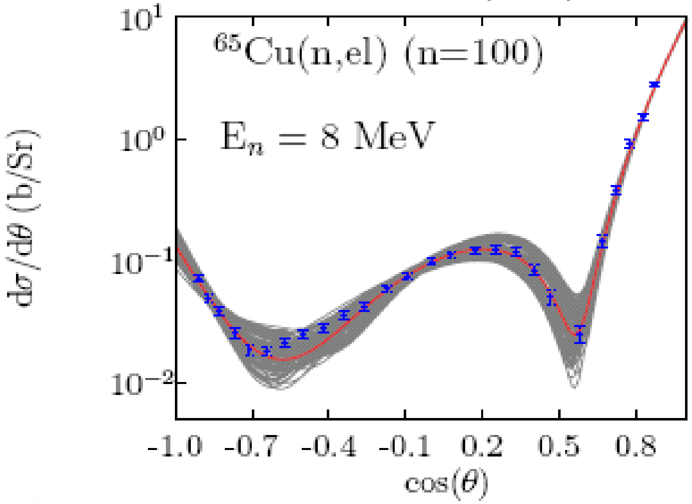


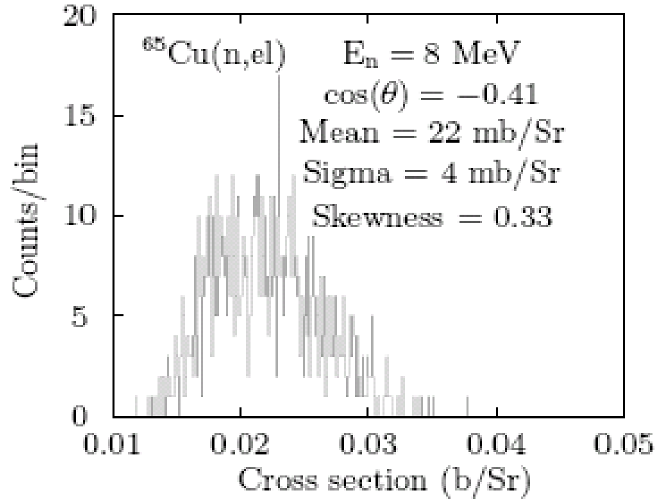


Uncertainties for Cu isotopes

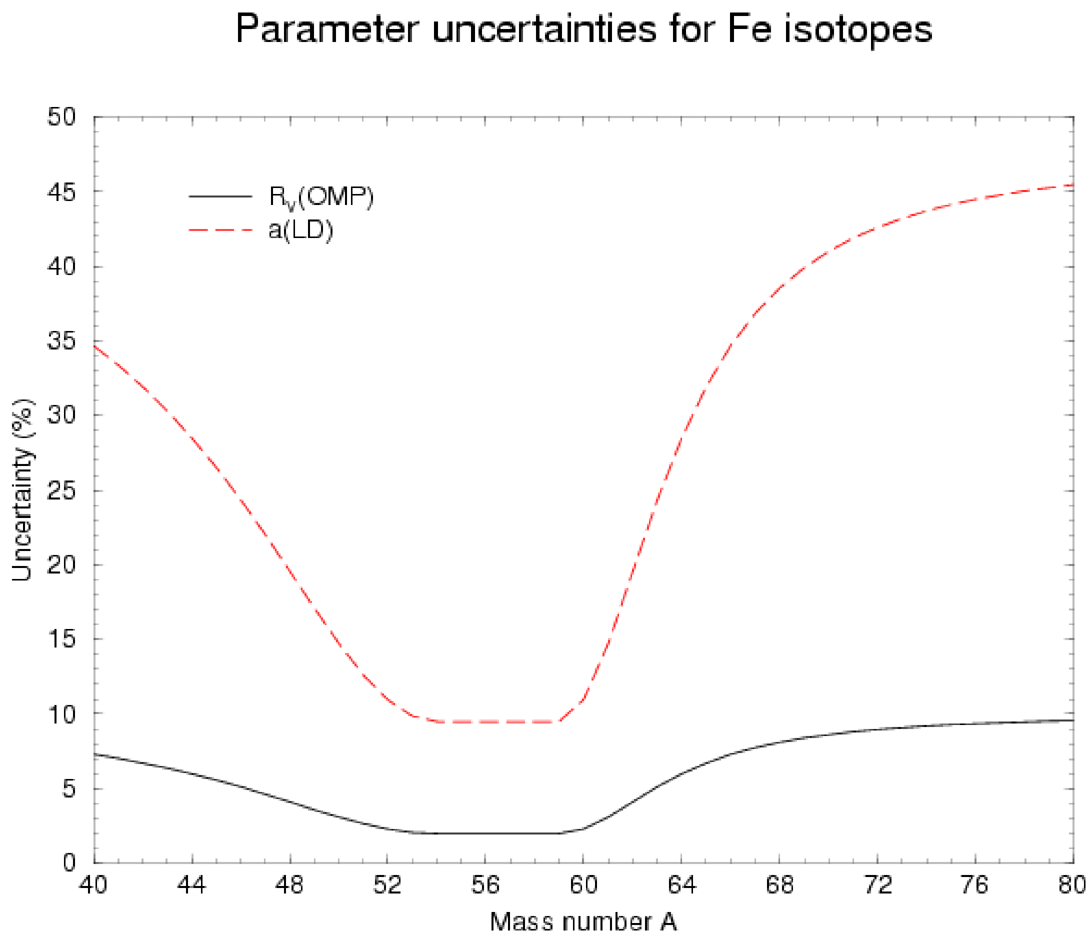


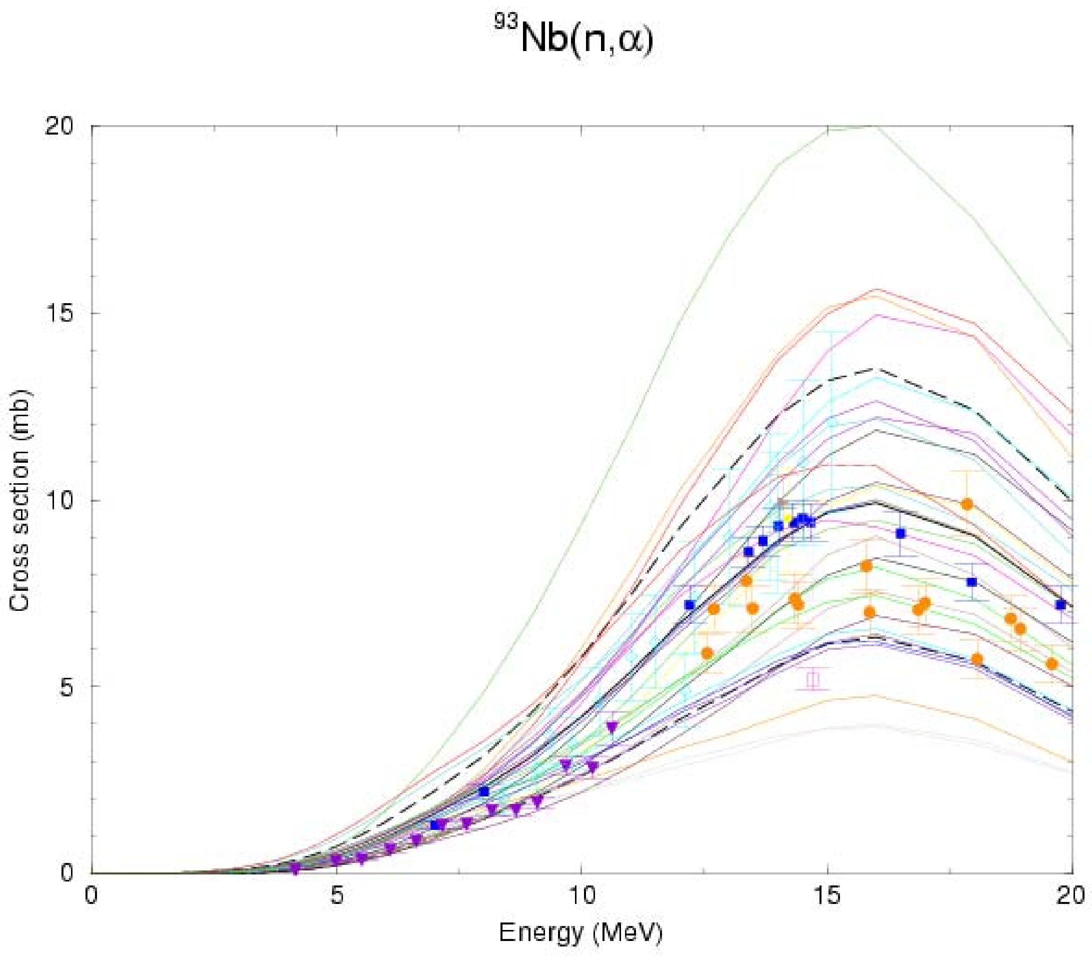




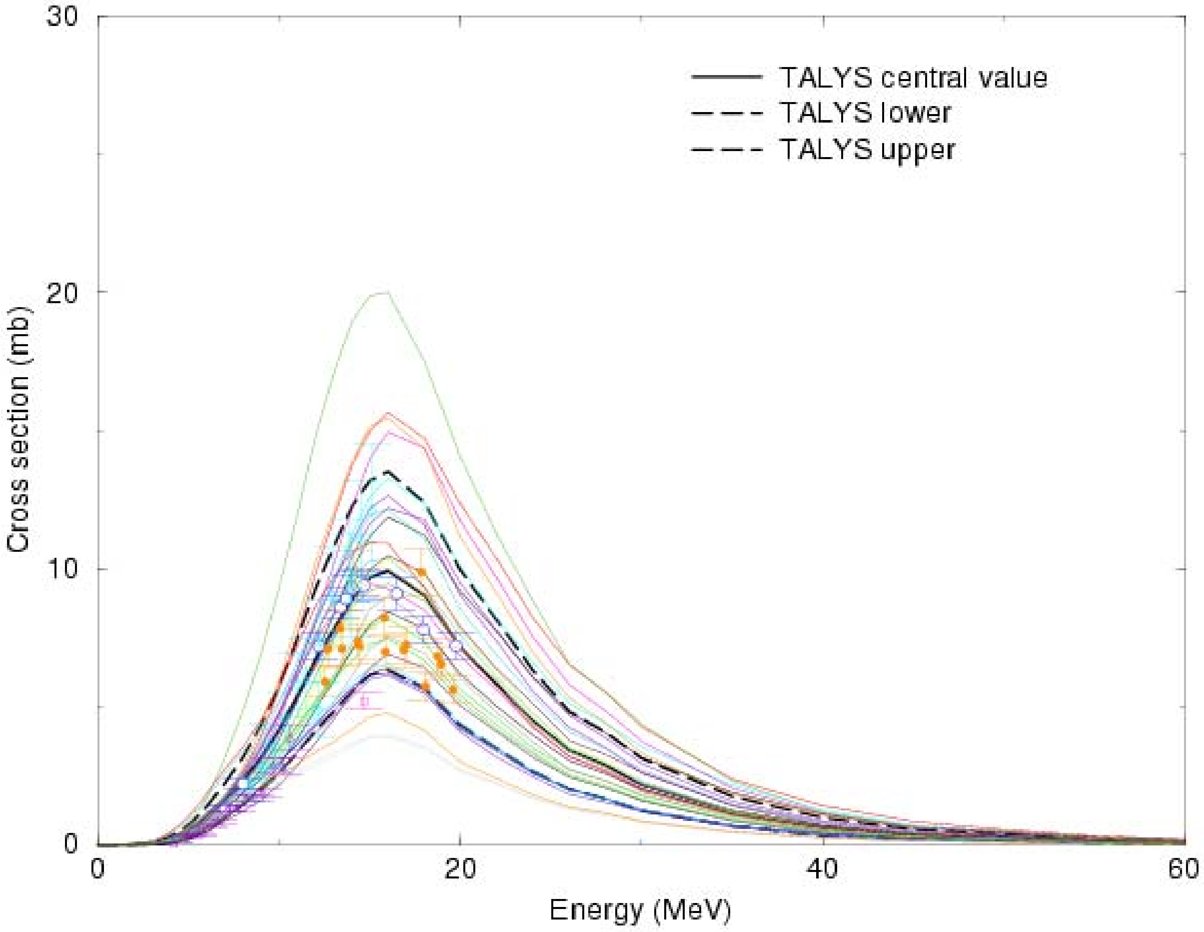


From stability to drip line



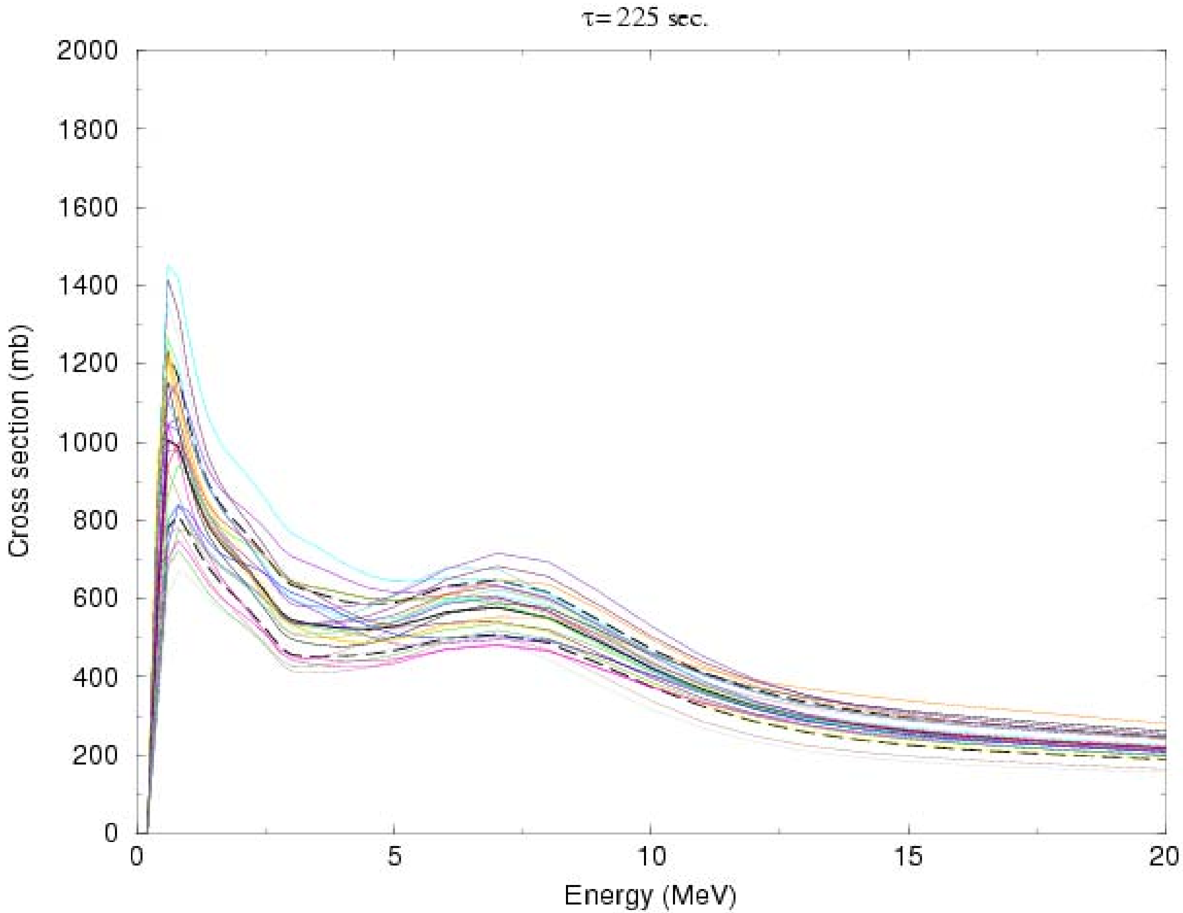

93Nb(n,α)
Cross section (mb)
Energy (MeV)
0
5
10
15
20
0
5
10
15
20

$^{93}Nb(n,\alpha)$



TALYS central value
TALYS lower
TALYS upper
Cross section (mb)
Energy (MeV)
0
10
20
30
0
20
40
60

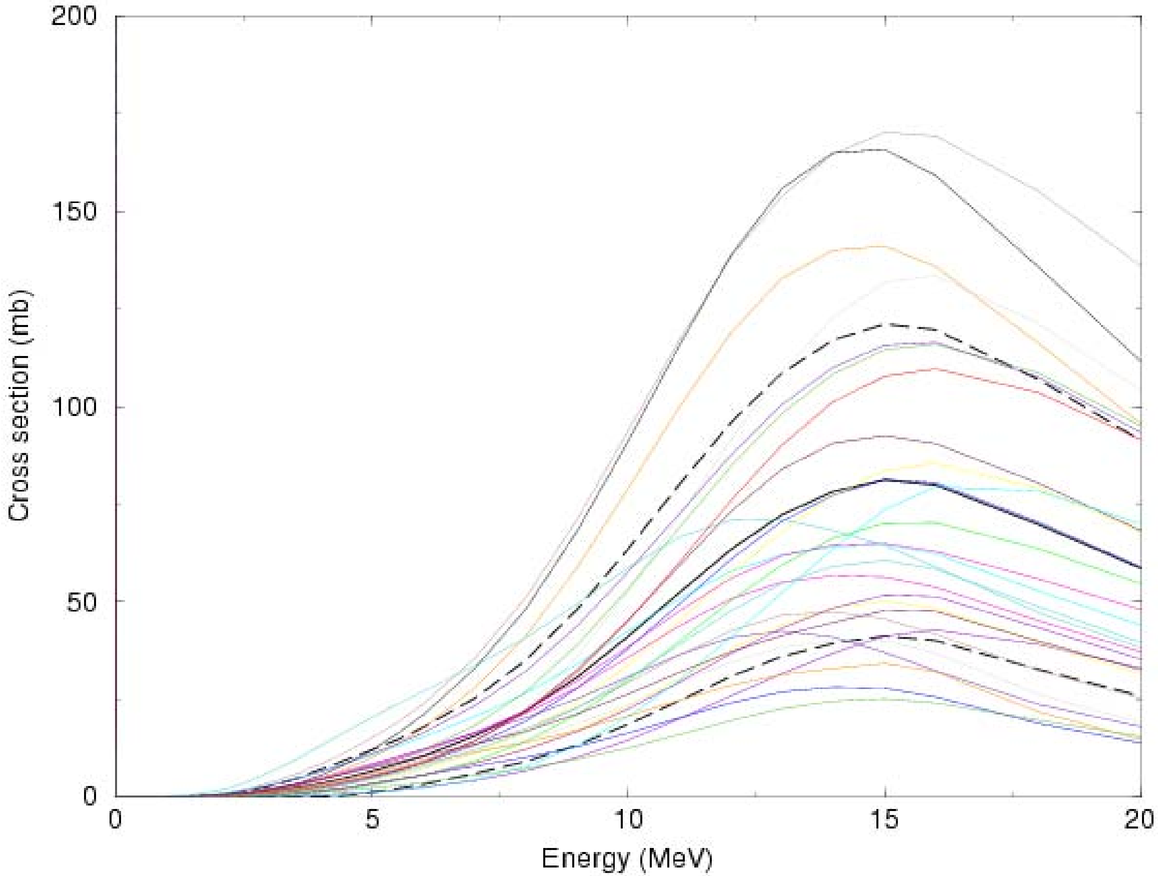
$^{87}Nb(n,n')$



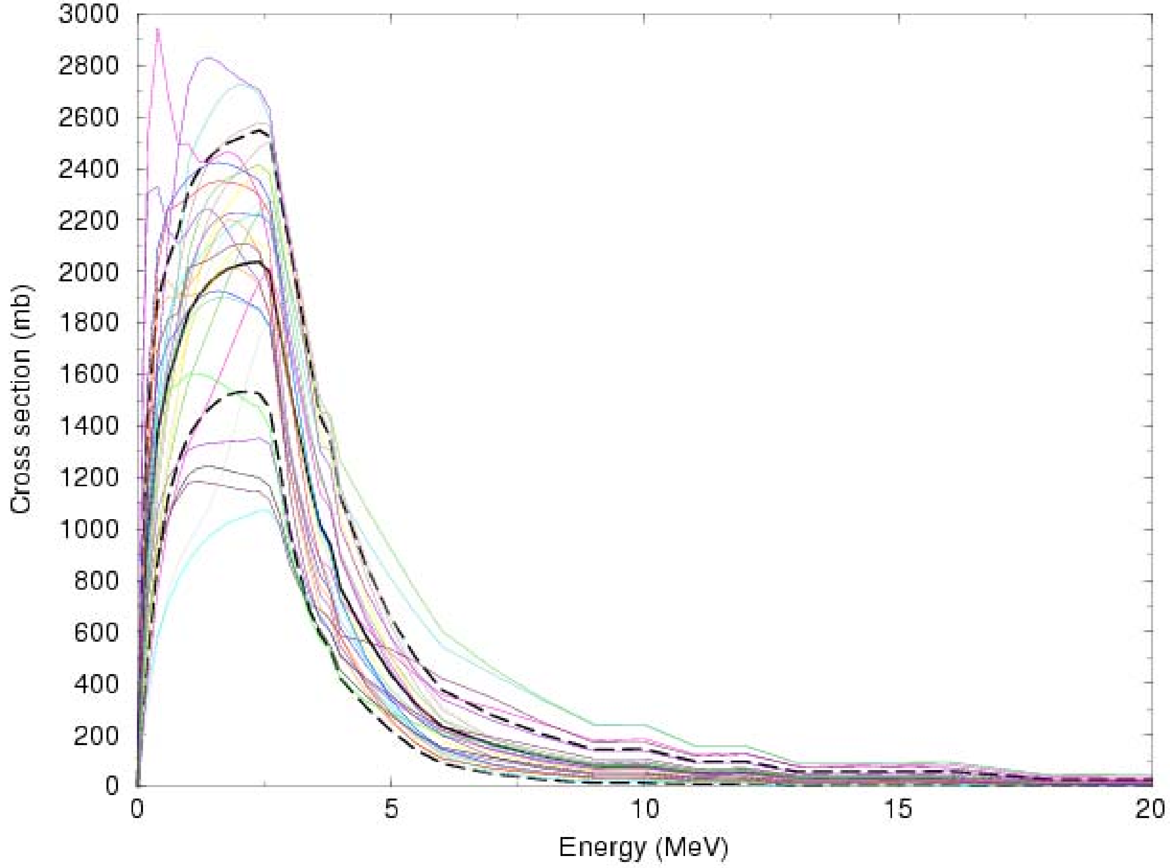
τ= 225 sec.
Cross section (mb)
0
200
400
600
800
1000
1200
1400
1600
1800
2000
0
5
10
15
20
Energy (MeV)

$^{87}Nb(n,\alpha)$

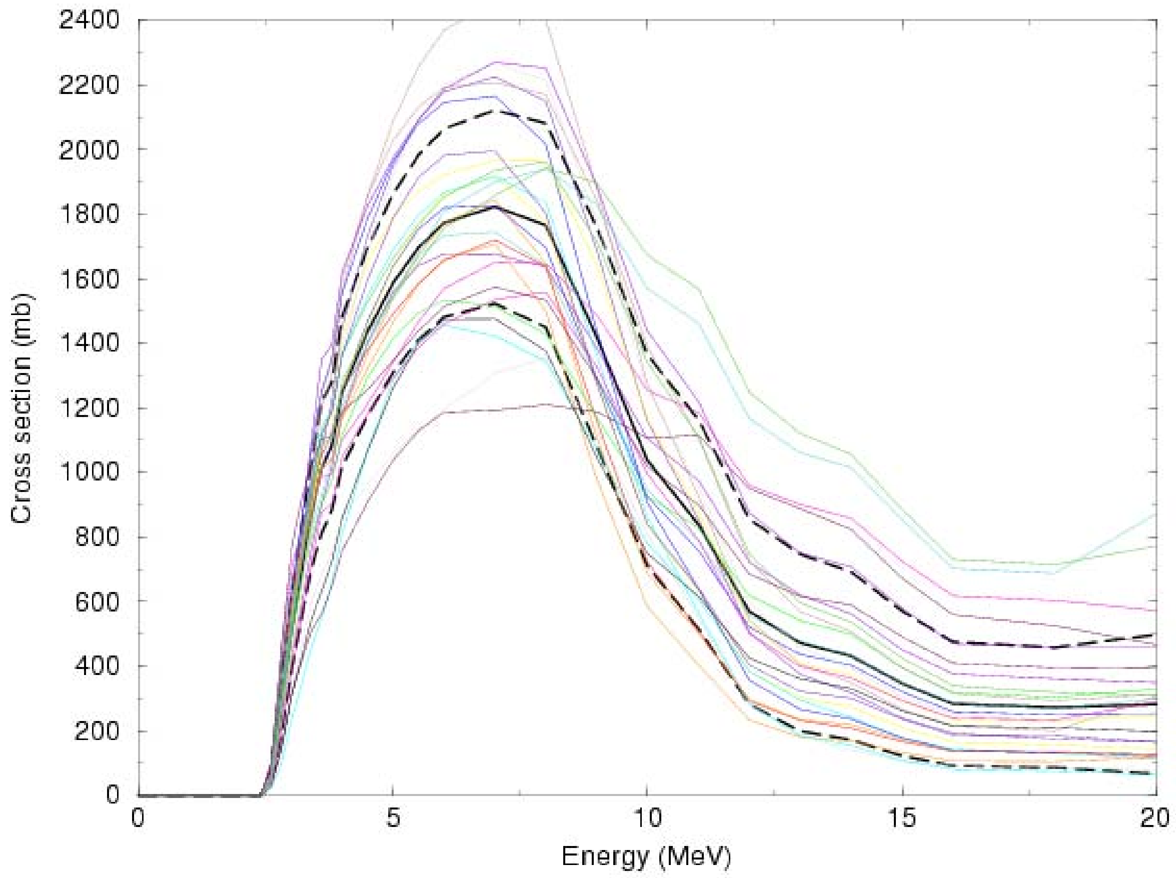
τ= 225 sec.



^{120}Nb(n,n')


3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
Cross section (mb)
0
5
10
15
20
Energy (MeV)

^{120}Nb(n,2n)



2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
Cross section (mb)
0
5
10
15
20
Energy (MeV)

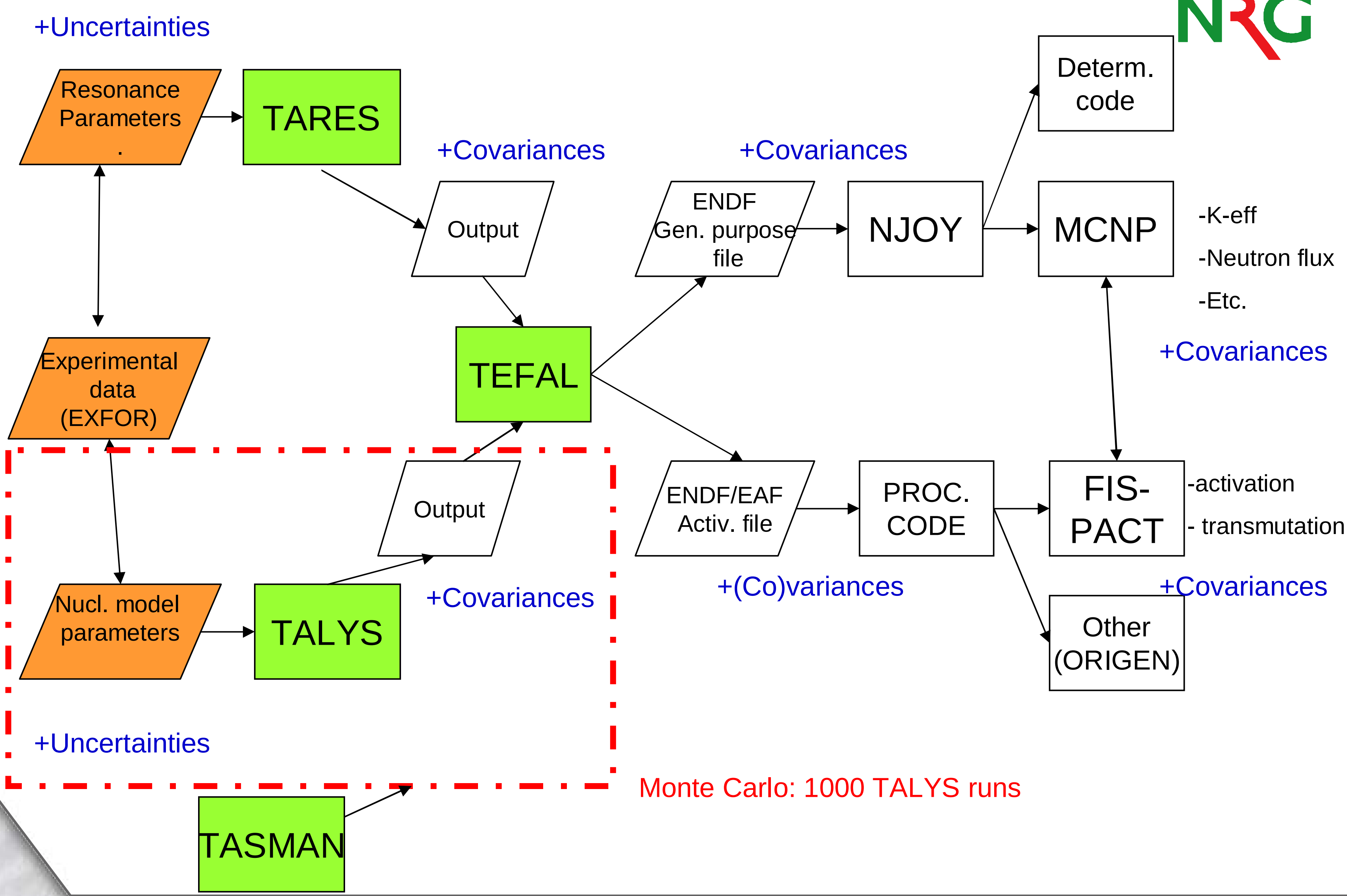
Uncertainties with Monte Carlo

Standard procedure (Don Smith):

- Determine uncertainty range for each nuclear model parameter
- Perform K(=1000) TALYS calculations with all parameters randomly sampled around their central values
- Various refinements possible:
  - Reject outlying results (leads to parameter correlations)
  - More precise inclusion of experimental data (Unified MC, D. Smith, H. Leeb), backward-forward MC (E. Bauge), etc.

All covariance data are now available: nuclear data libraries can be filled!

Nuclear data scheme + covariances



Application 1: TENDL

TALYS Evaluated Nuclear Data Library, www.talys.eu/tendl2009

- n, p, d, t ,h, a and g libraries in ENDF-6 format
- 2400 nuclides (all with lifetime > 1 sec.) up to 200 MeV
- **Neutrons: complete covariance data (MF31-MF35)**
- MCNP-libraries (n,p and d) and multi-group covariances (n only)
- Production time: 2 months (40 processors)

Strategy:

- Always ensure completeness, global improvement in 2010, 2011..
- Extra effort for important nuclides, especially when high precision is required (e.g. actinides): adjusted parameters (data fitting). **These input files per nuclide are stored for future use**.
- All libraries are always reproducible from scratch
- The ENDF-6 libraries are created, not manually touched
- **Zeroing in on the truth for the whole nuclide chart at once**

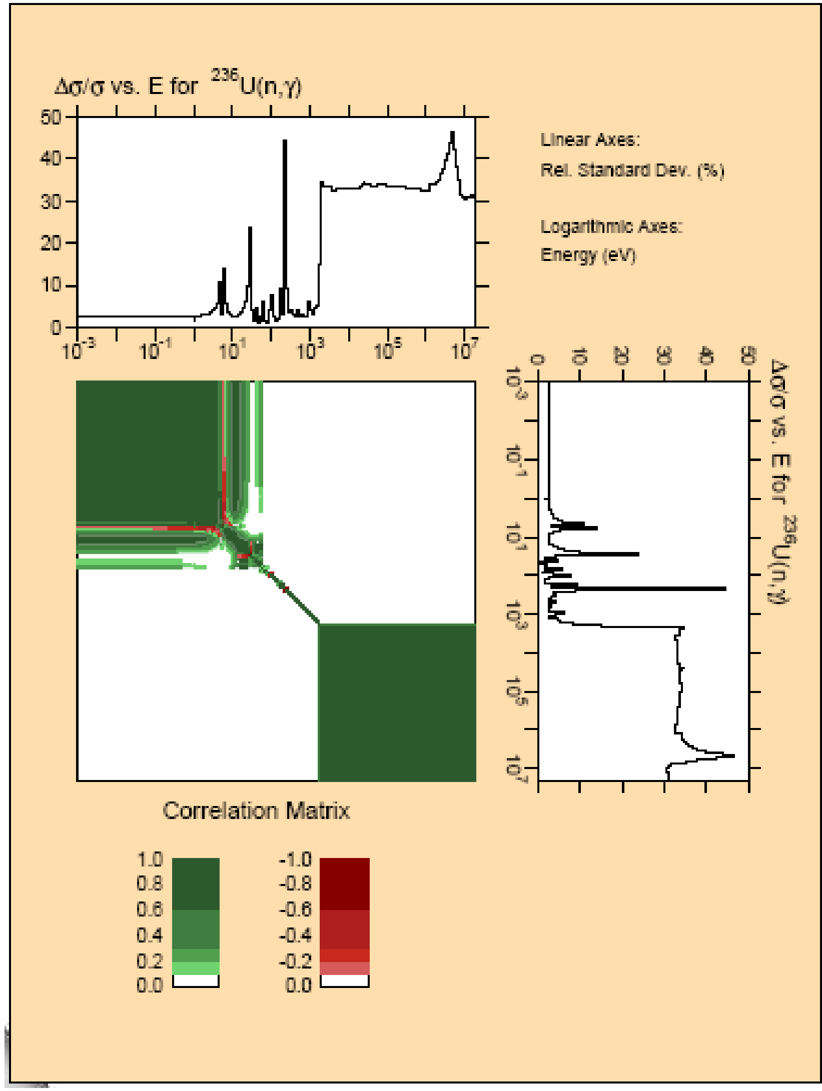
TENDL: Complete ENDF-6 data libraries

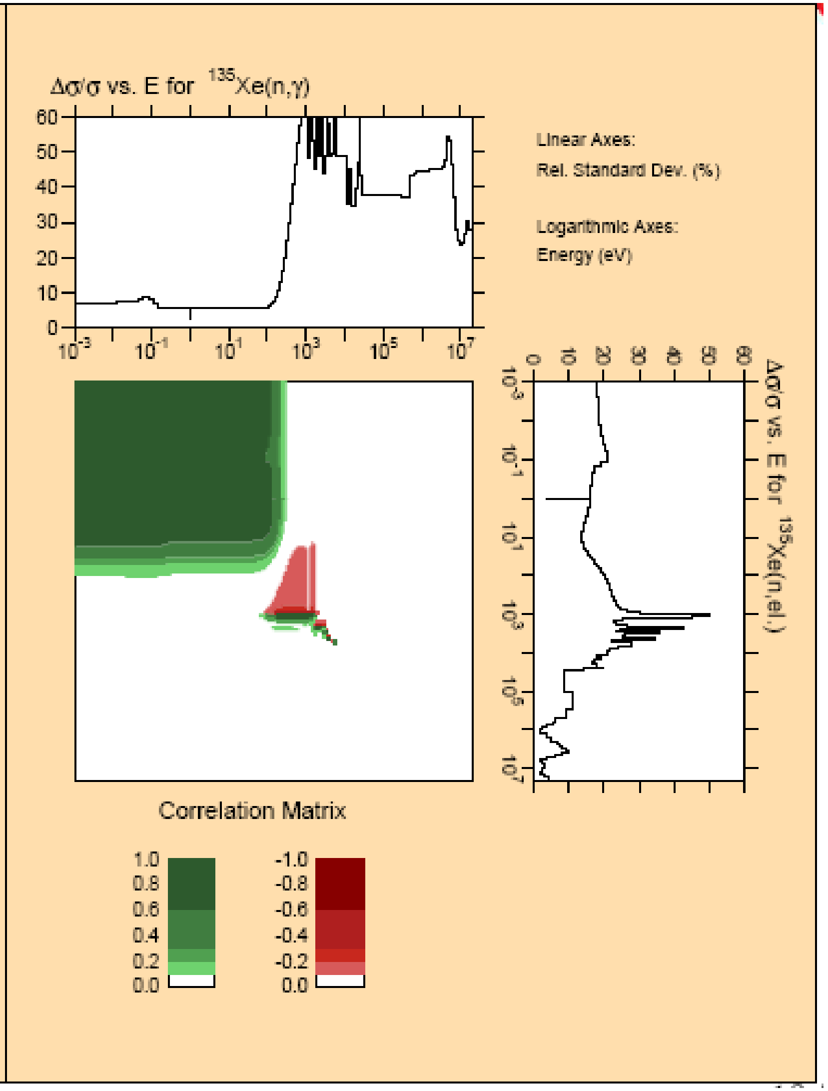
MF1: description and average fission quantities
MF2: resonance data
MF3: cross sections
MF4: angular distributions
MF5: energy spectra
MF6: double-differential spectra, particle yields and residual products
MF8-10: isomeric cross sections and ratios
MF12-15: gamma yields, spectra and angular distributions

Covariance data

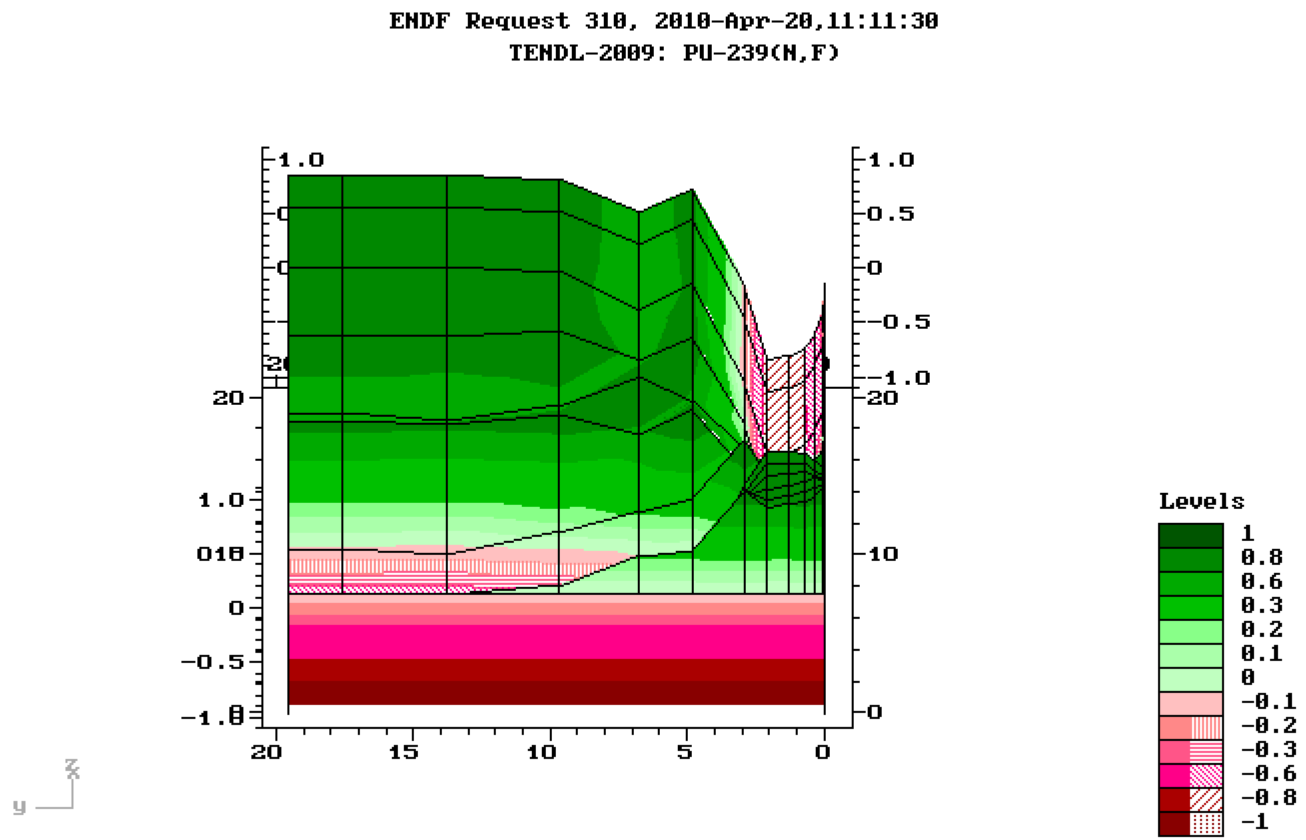
MF31: covariances of average fission quantities (TENDL-2010)
MF32: covariances of resonance parameters
MF33: covariances of cross sections
MF34: covariances of angular distributions
MF35: covariances of fission neutron spectra (TENDL-2010) and particle spectra (TENDL-2011)
MF40: covariances of isomeric data (TENDL-2011)

Covariance plots (NJOY)



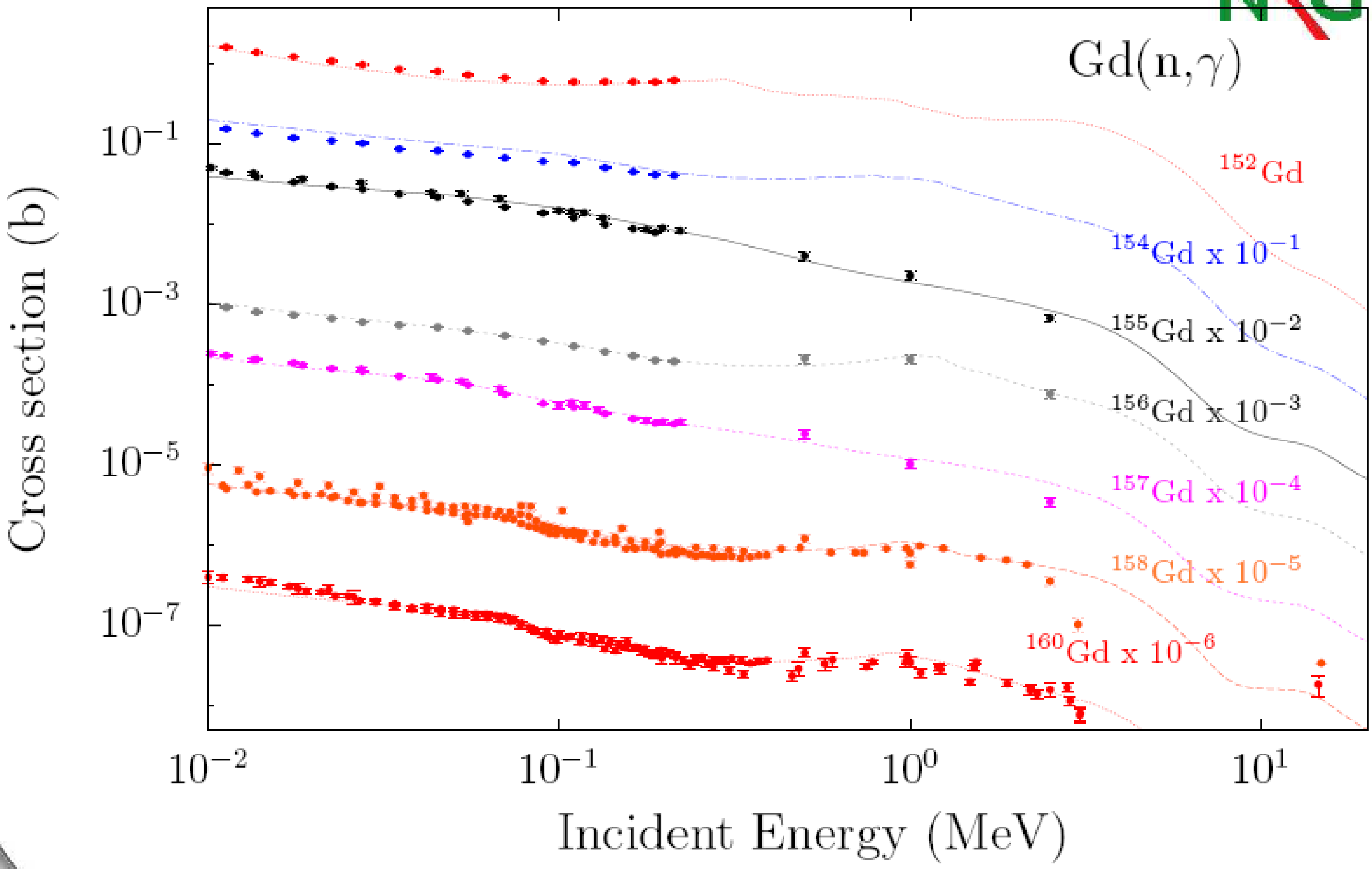


IAEA covariance visualisation system (V. Zerkin)



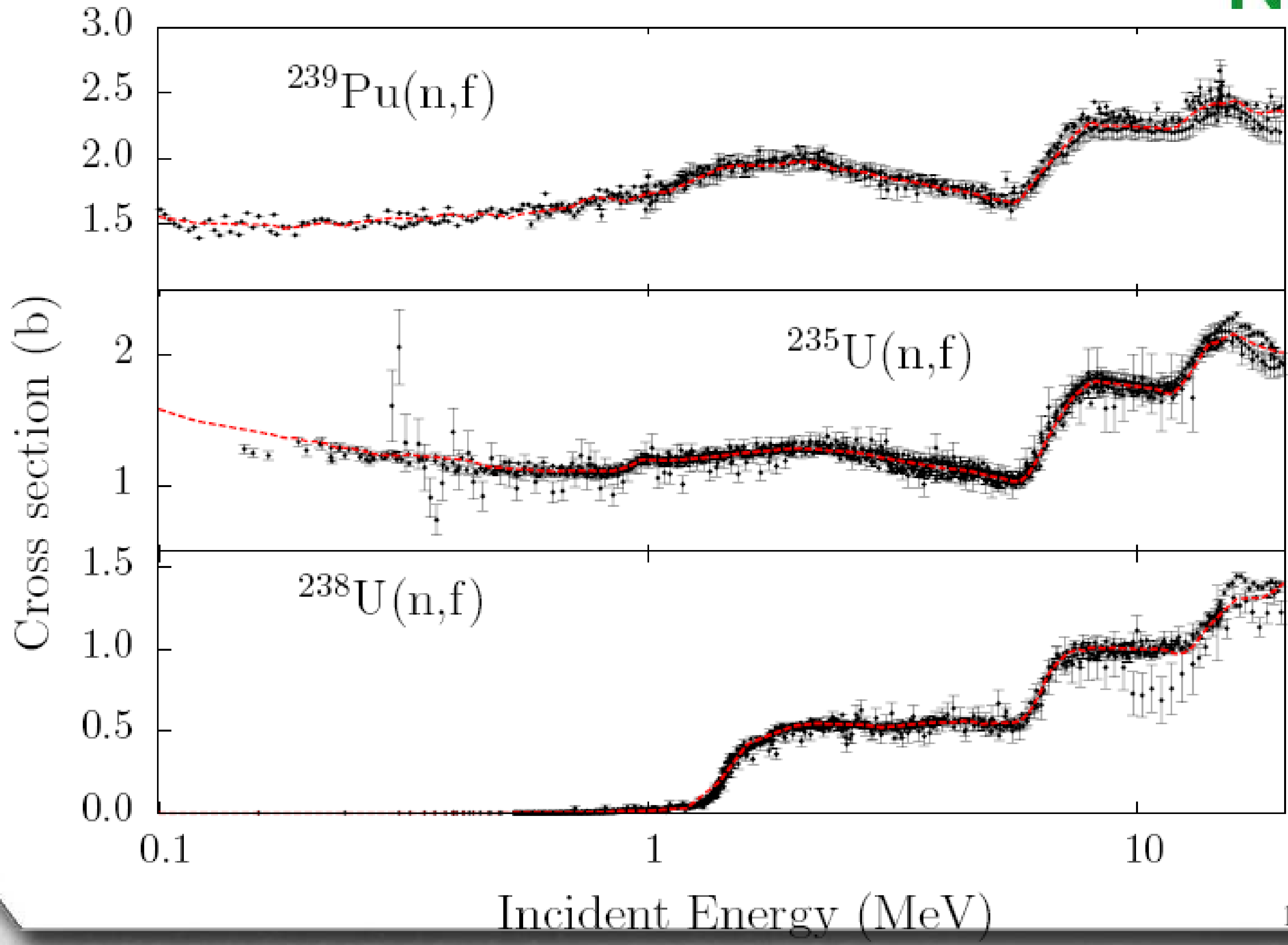
Examples 1: Gadolinium isotopes

23:17:11

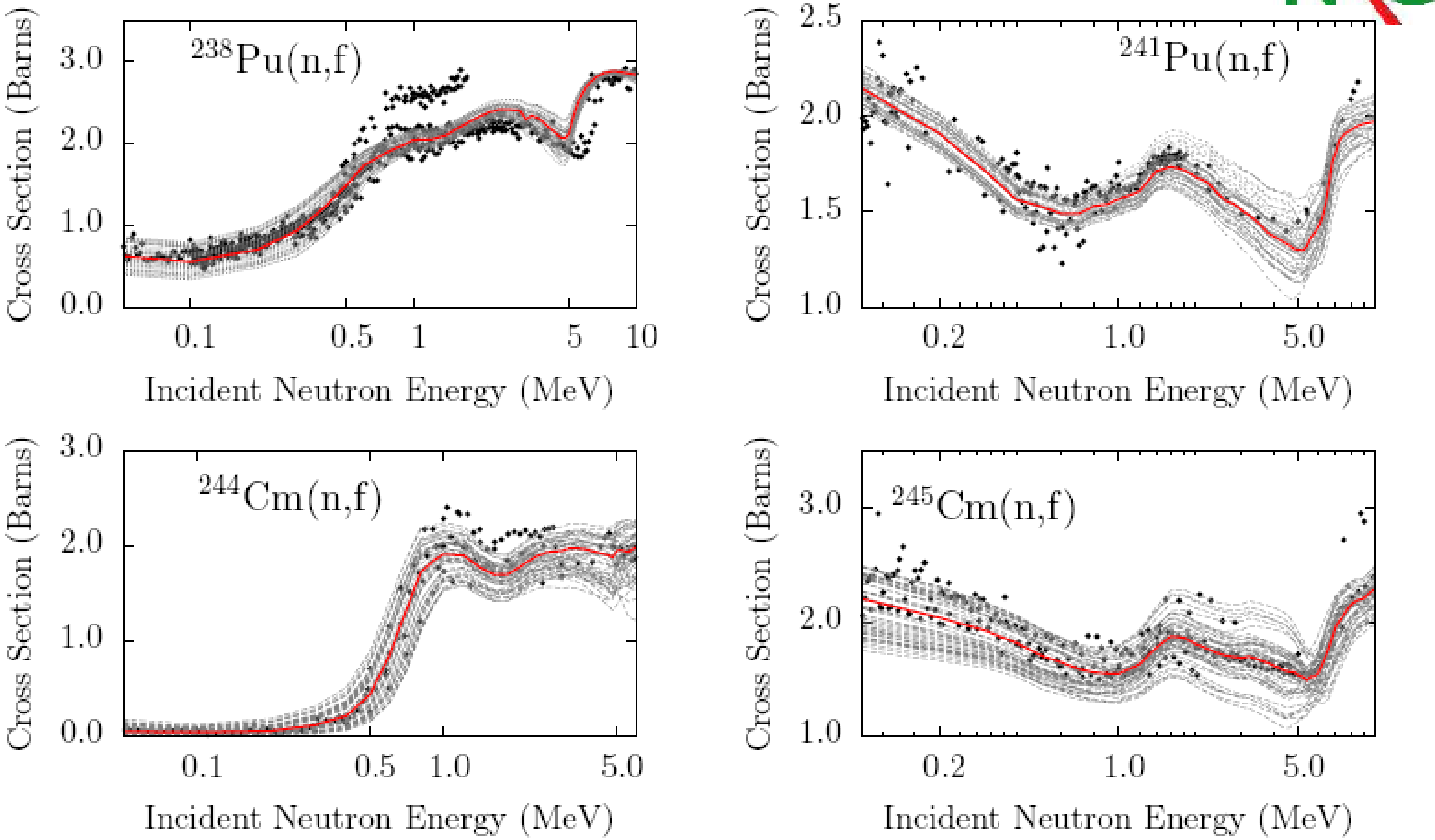


Examples 3: Some actinides

23:18:45



Covariances: example



Application 2: "Total" Monte Carlo

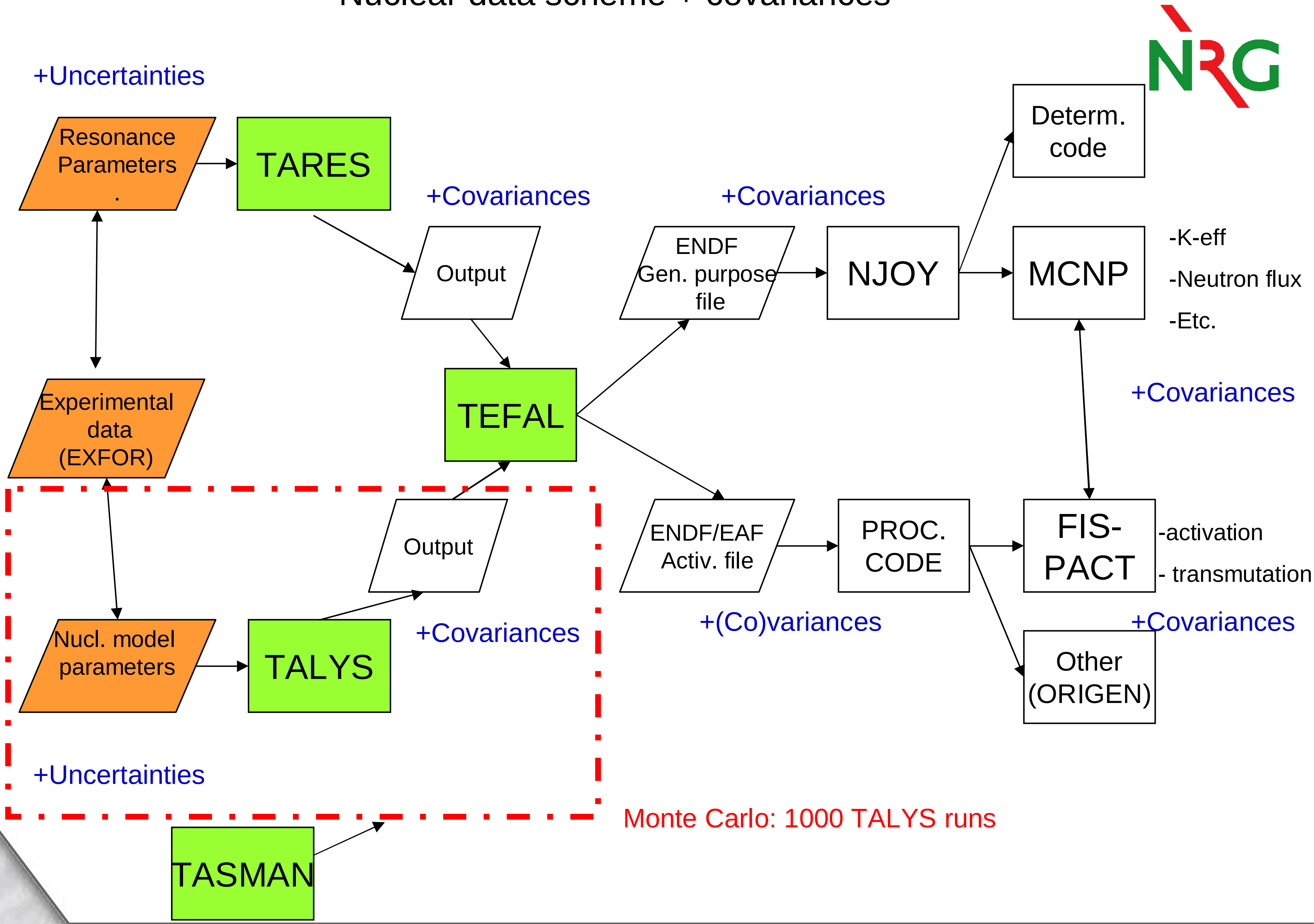
- Propagating covariance data is an approximation of true uncertainty propagation (especially regarding ENDF-6 format limitations)
- Covariance data requires extra processing and "satellite software" for application codes
- Alternative: Create an ENDF-6 file for each random sample and finish the entire physics-to-application loop. (Koning and Rochman, Ann Nuc En 35, 2024 (2008)

> *"Researchers should cease trying to be clever in devising refinements to old methods that were developed when computational resources were limited.*
> *Instead, their creative instincts should be redirected to unleashing the full potential of computers for* **brute** *force analysis"*

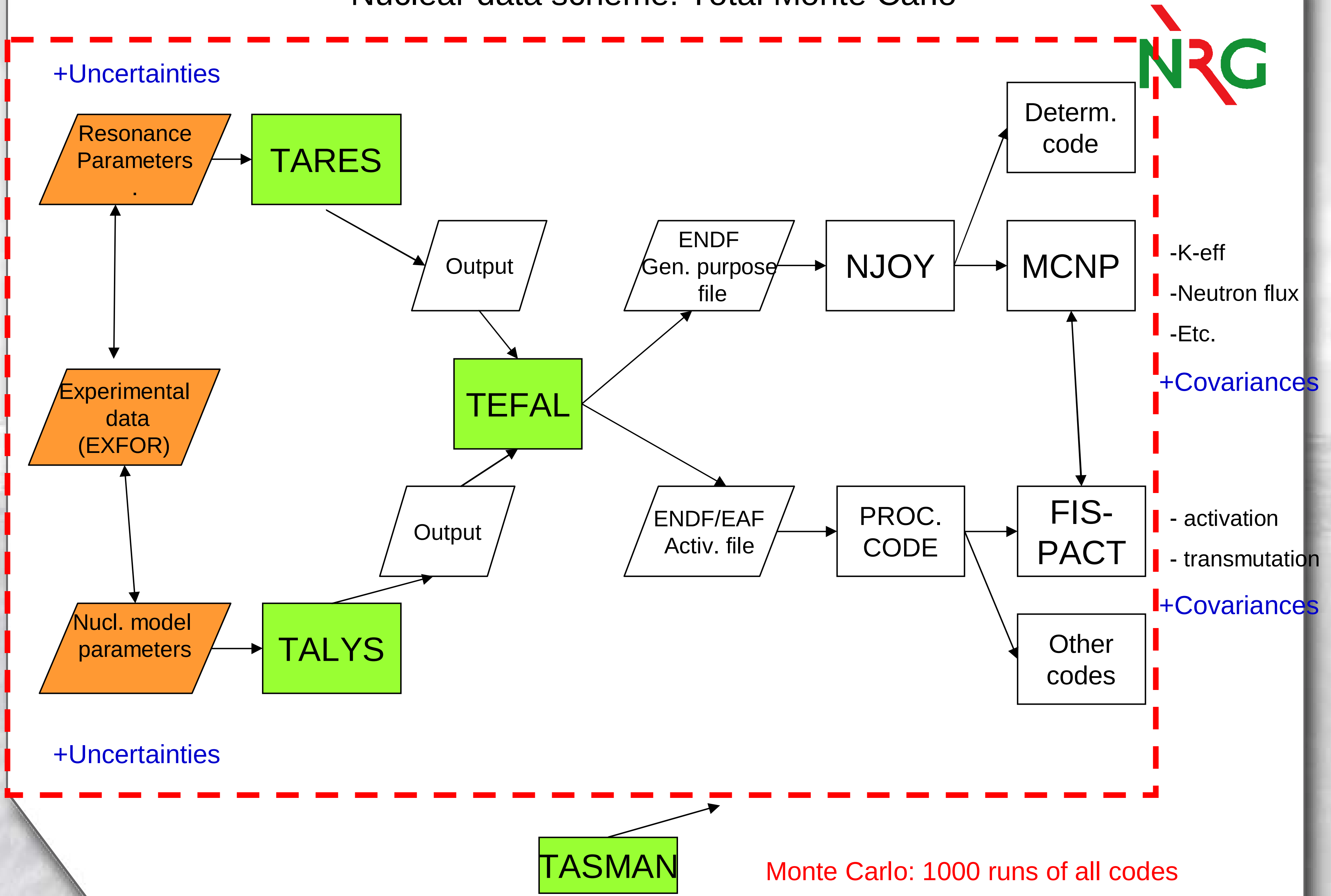
D. Smith, Santa Fe 2004

Do one brave thing today, then run like hell!

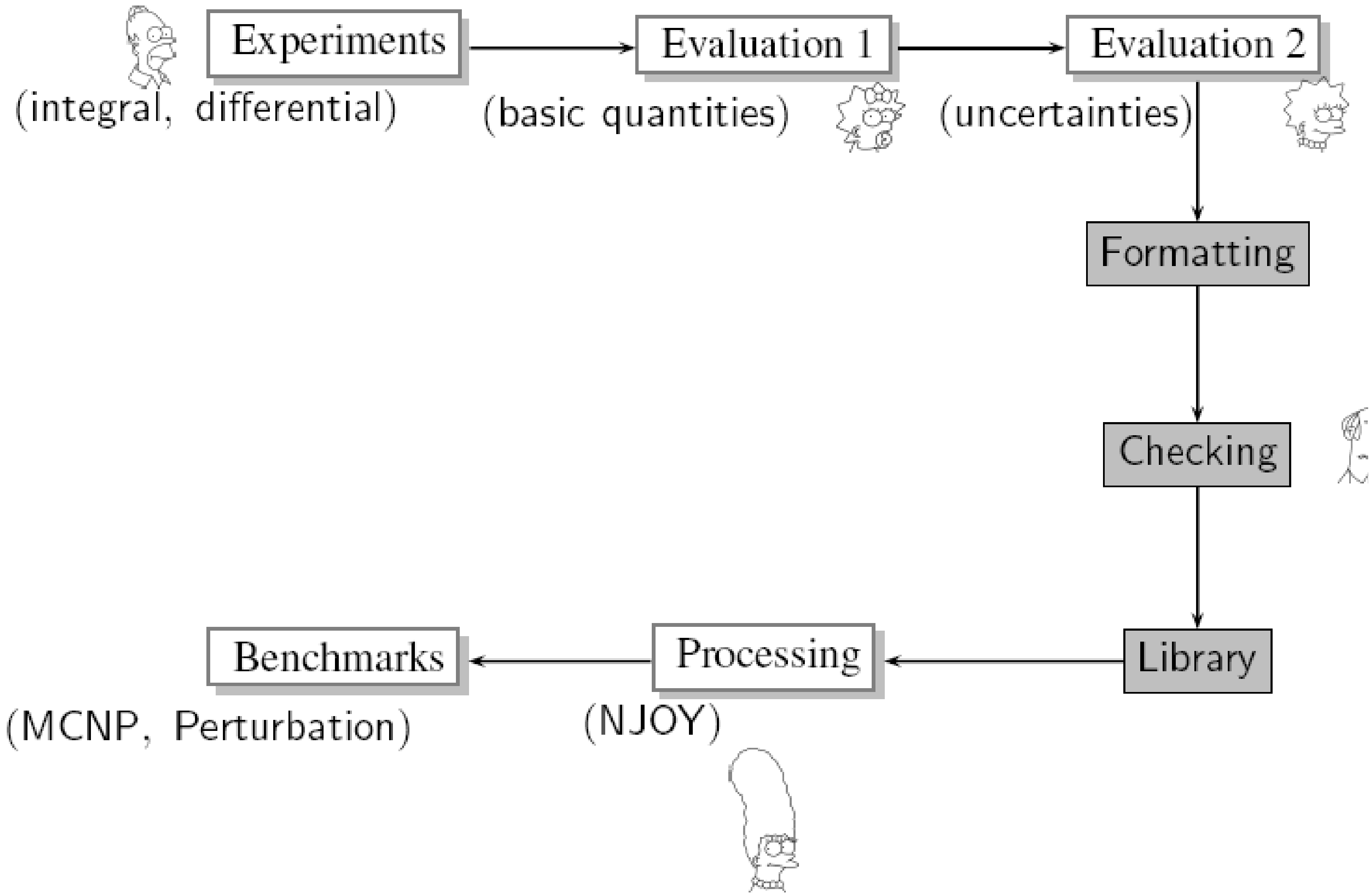
Nuclear data scheme + covariances



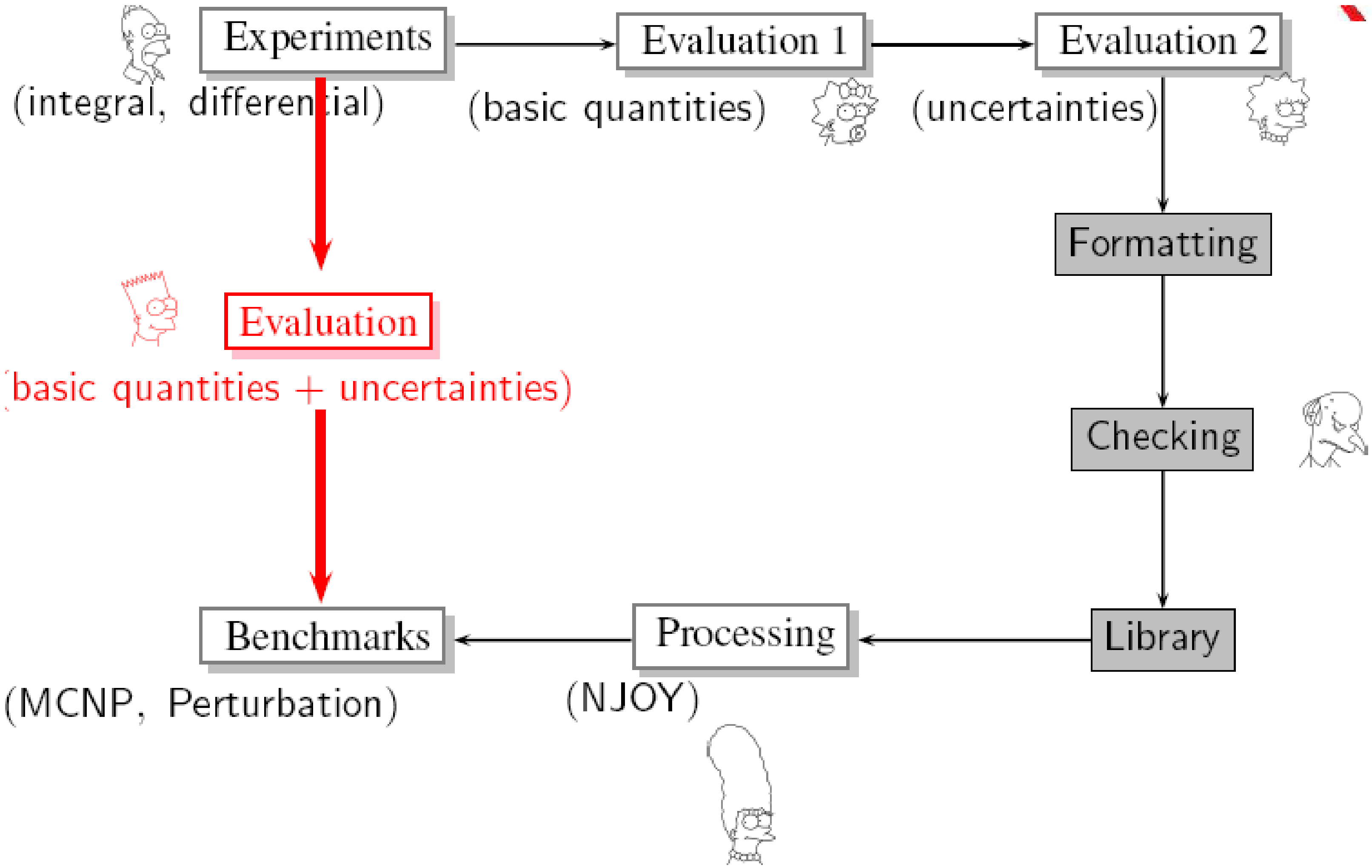
Nuclear data scheme: Total Monte Carlo



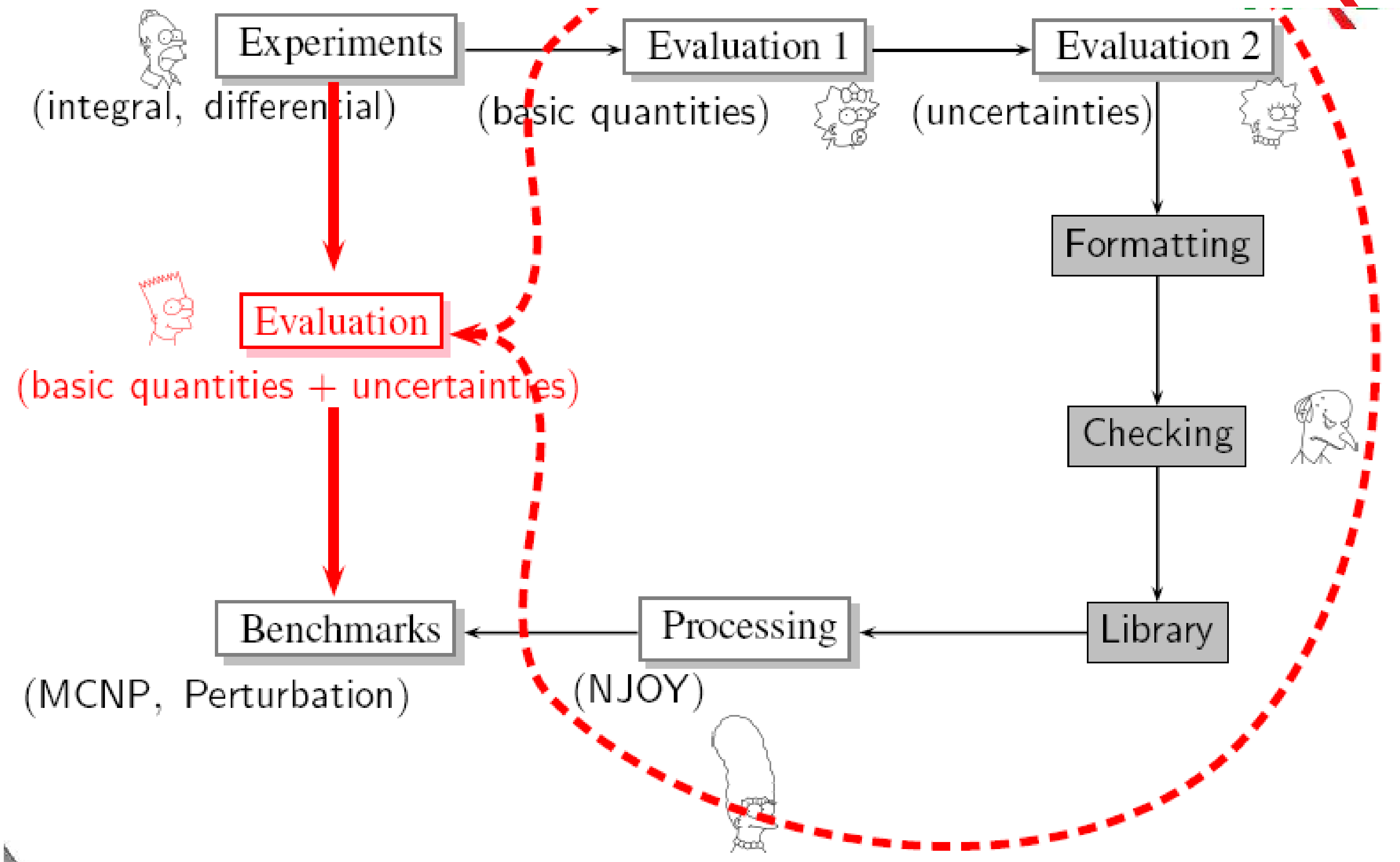
Systematic nuclear data evaluation



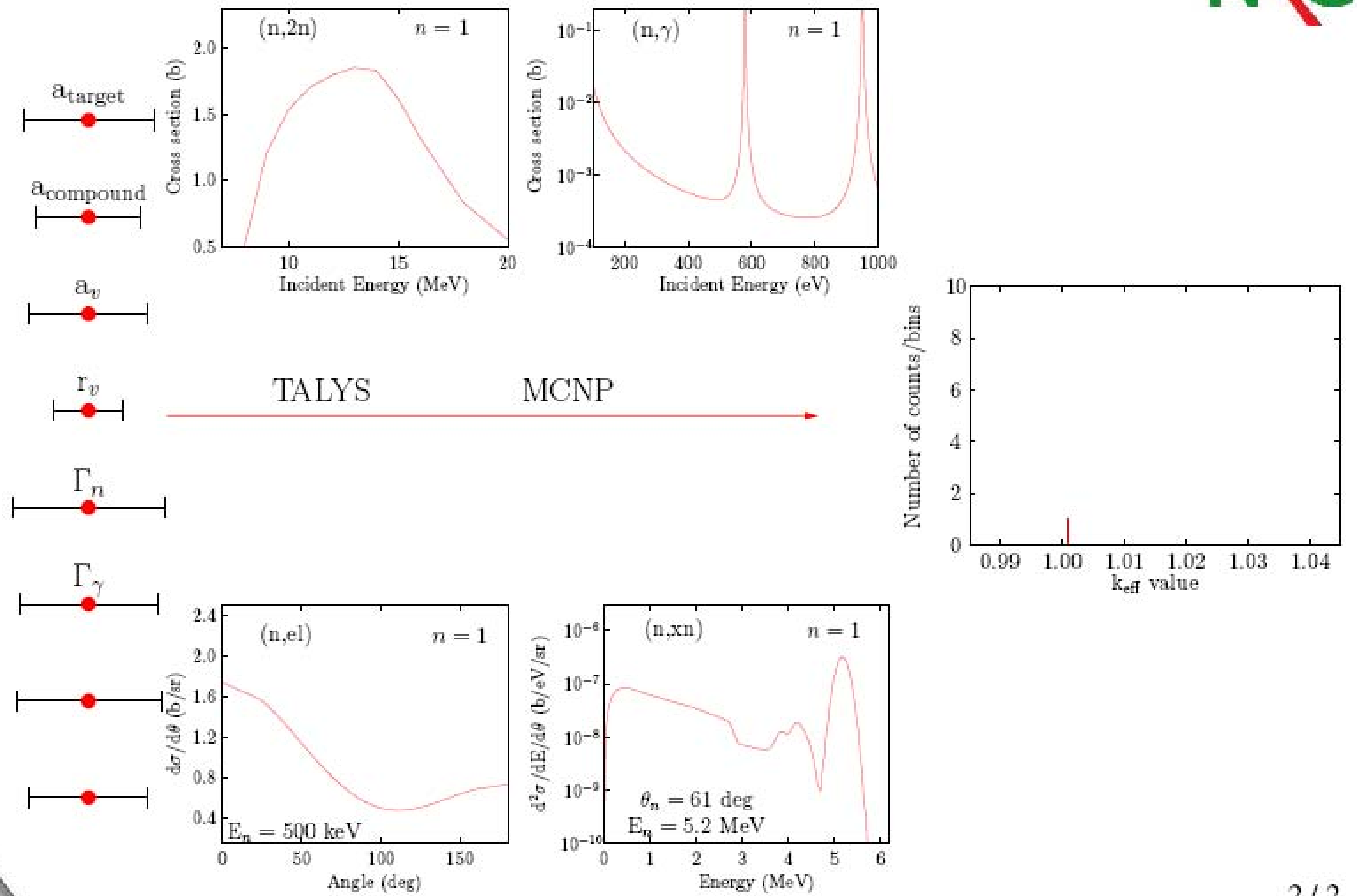
Systematic nuclear data evaluation



Systematic nuclear data evaluation



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



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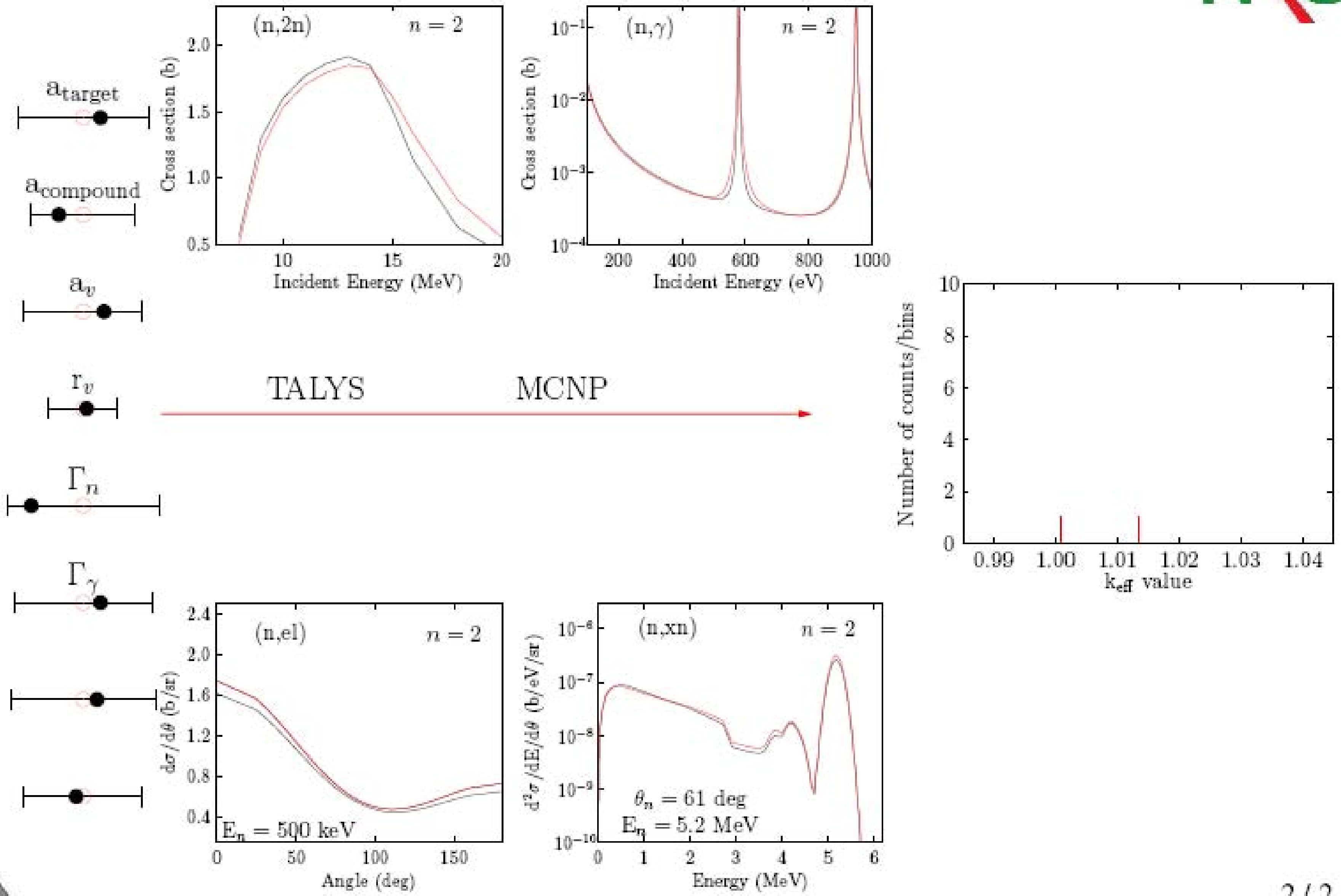

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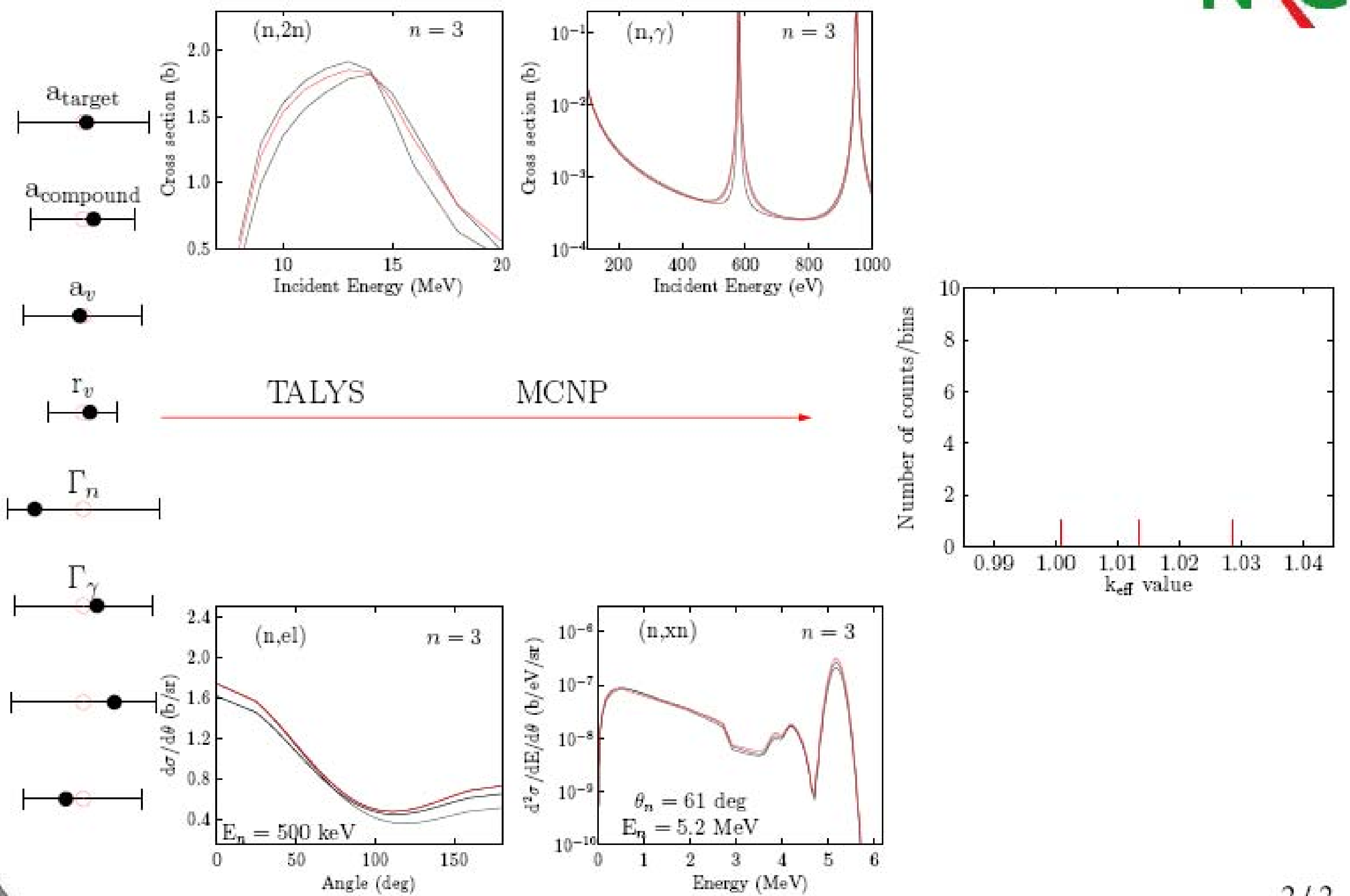

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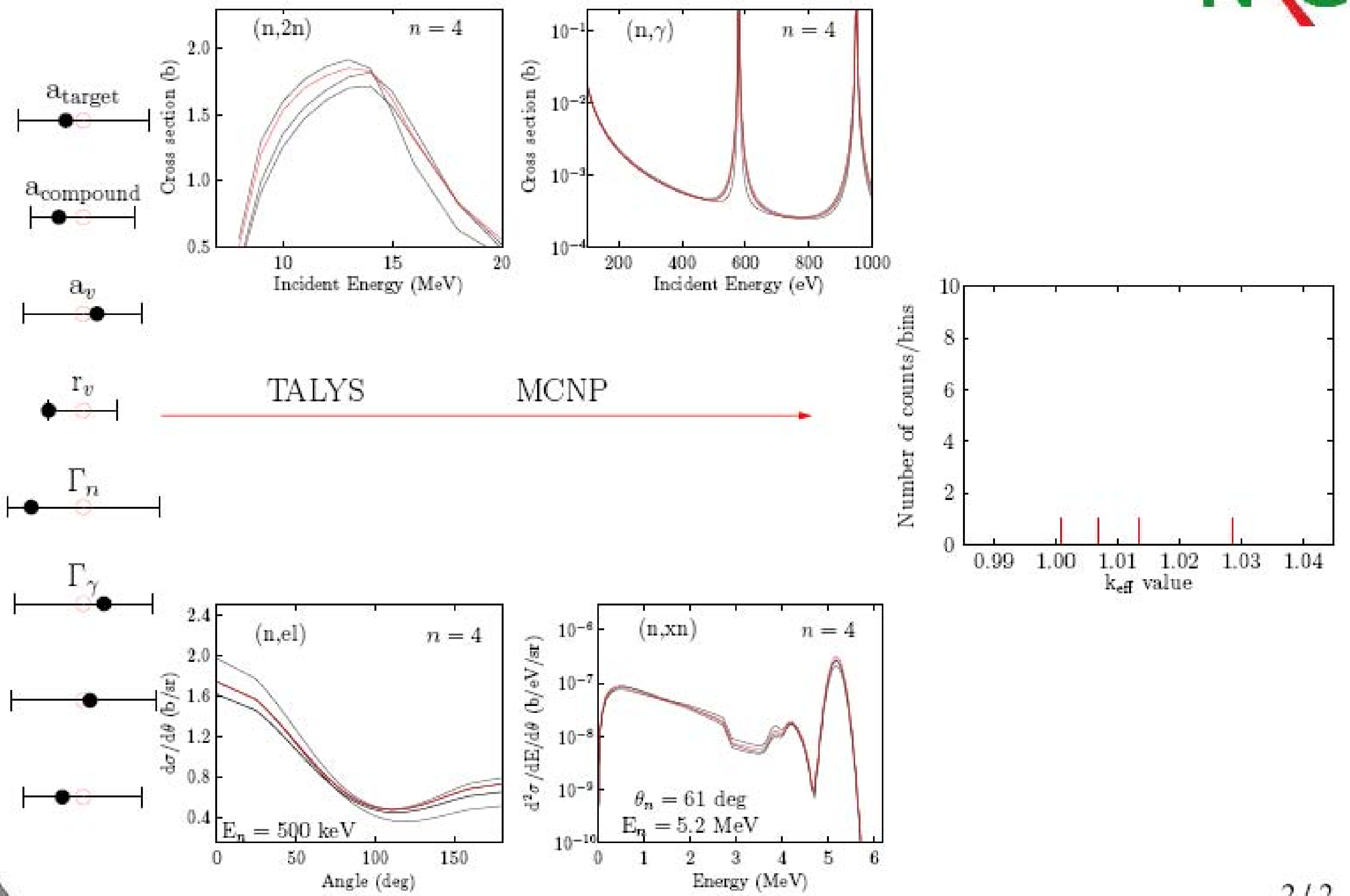
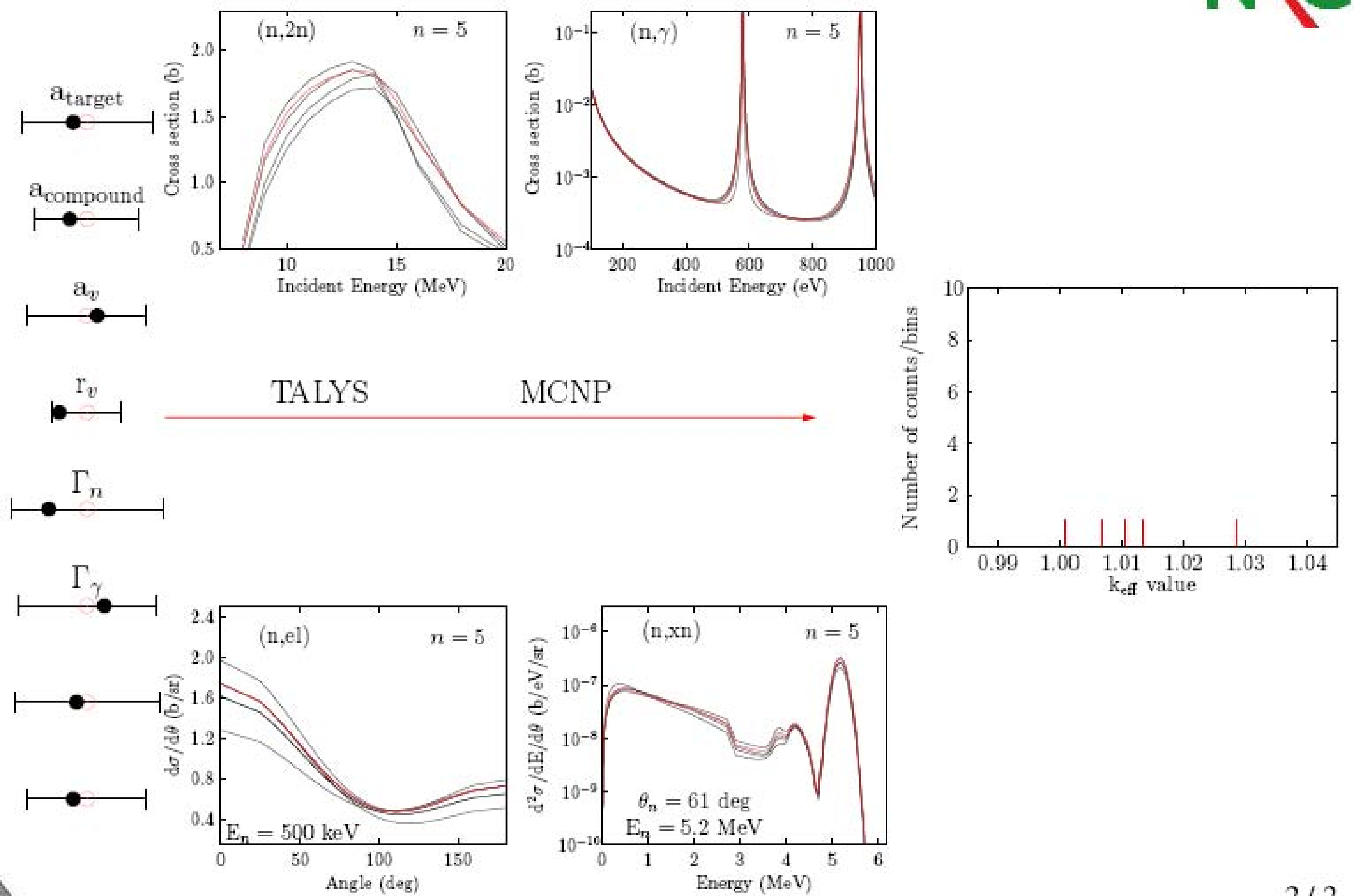
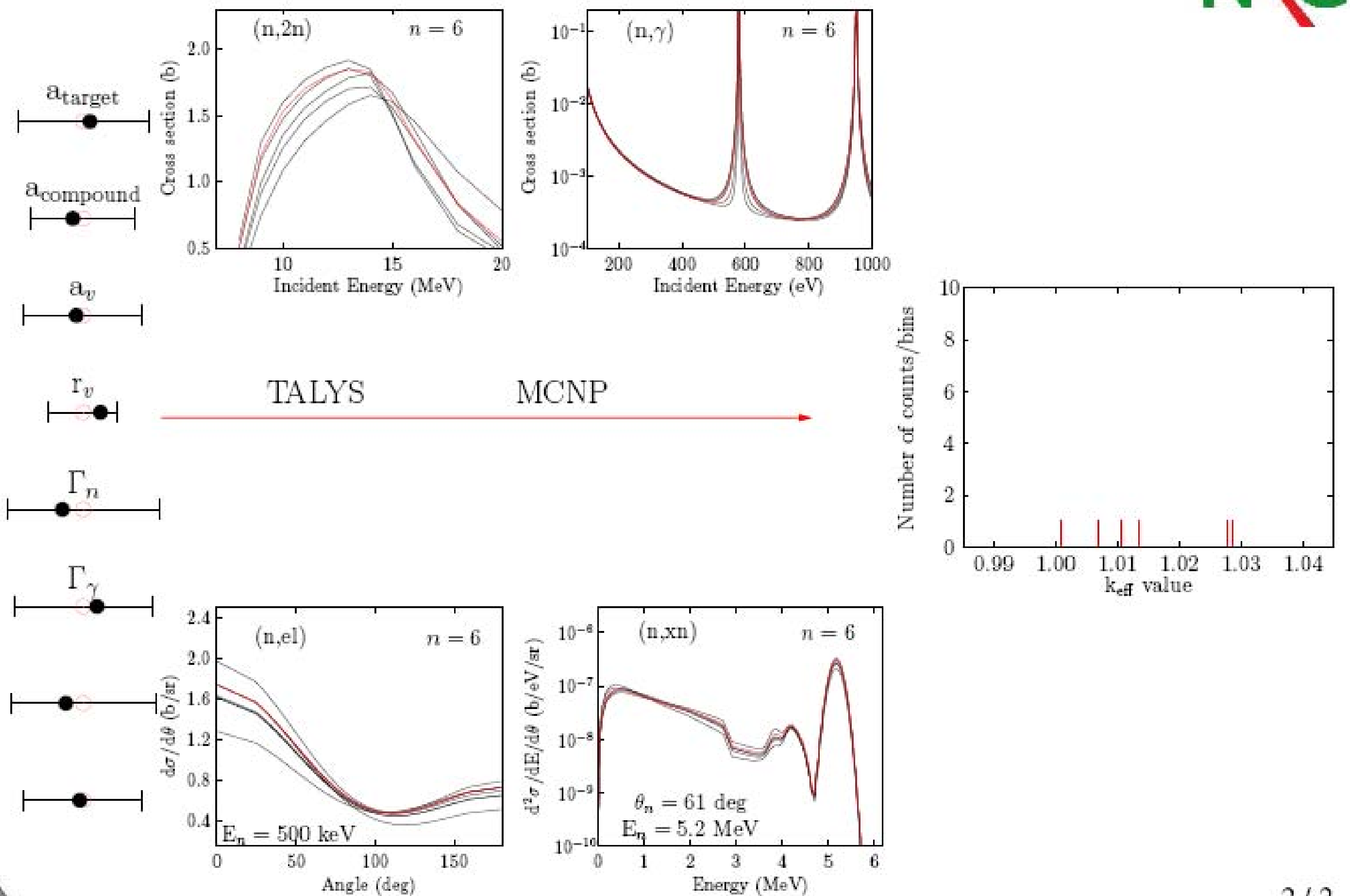


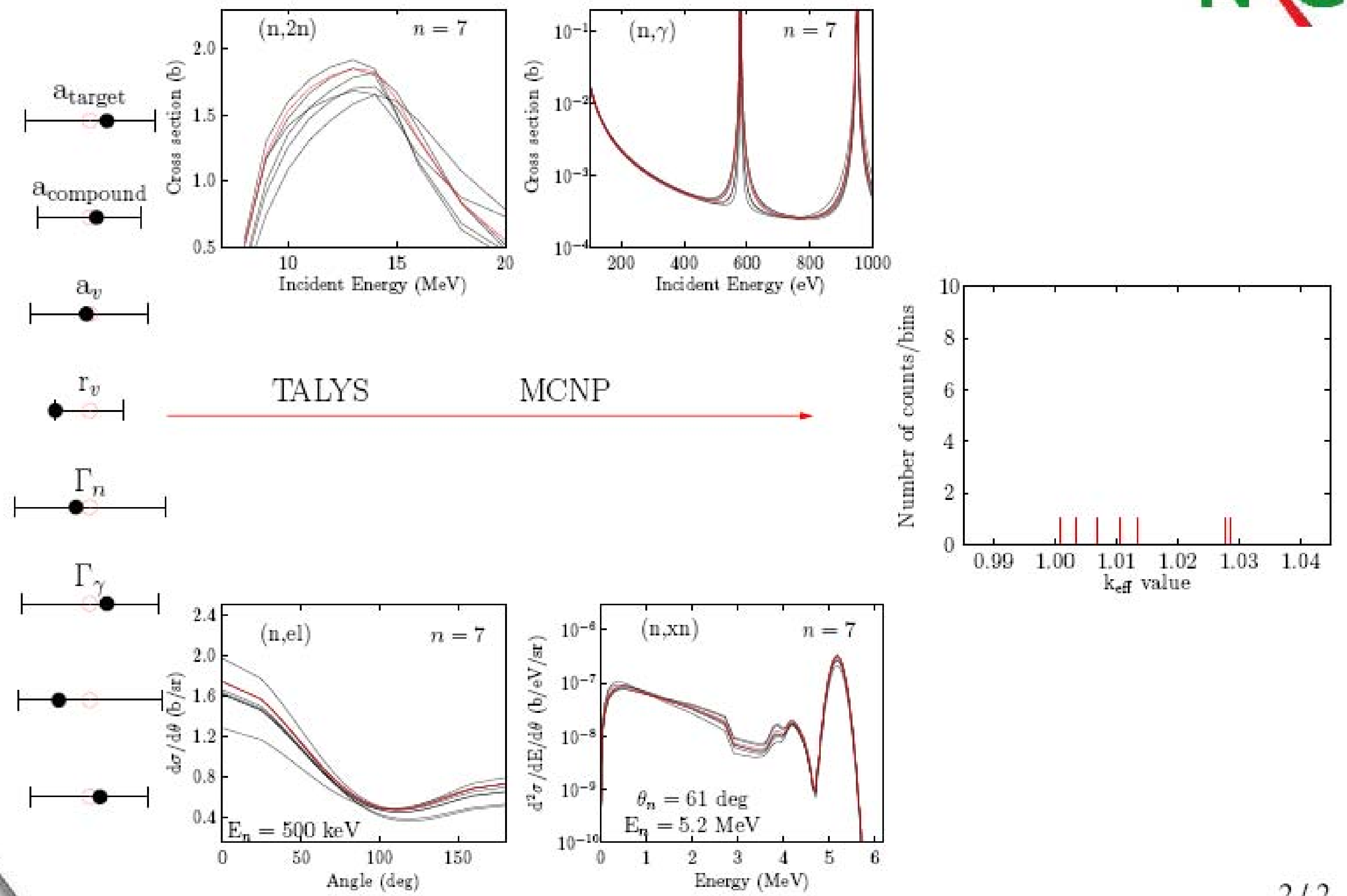
“1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb”



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



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



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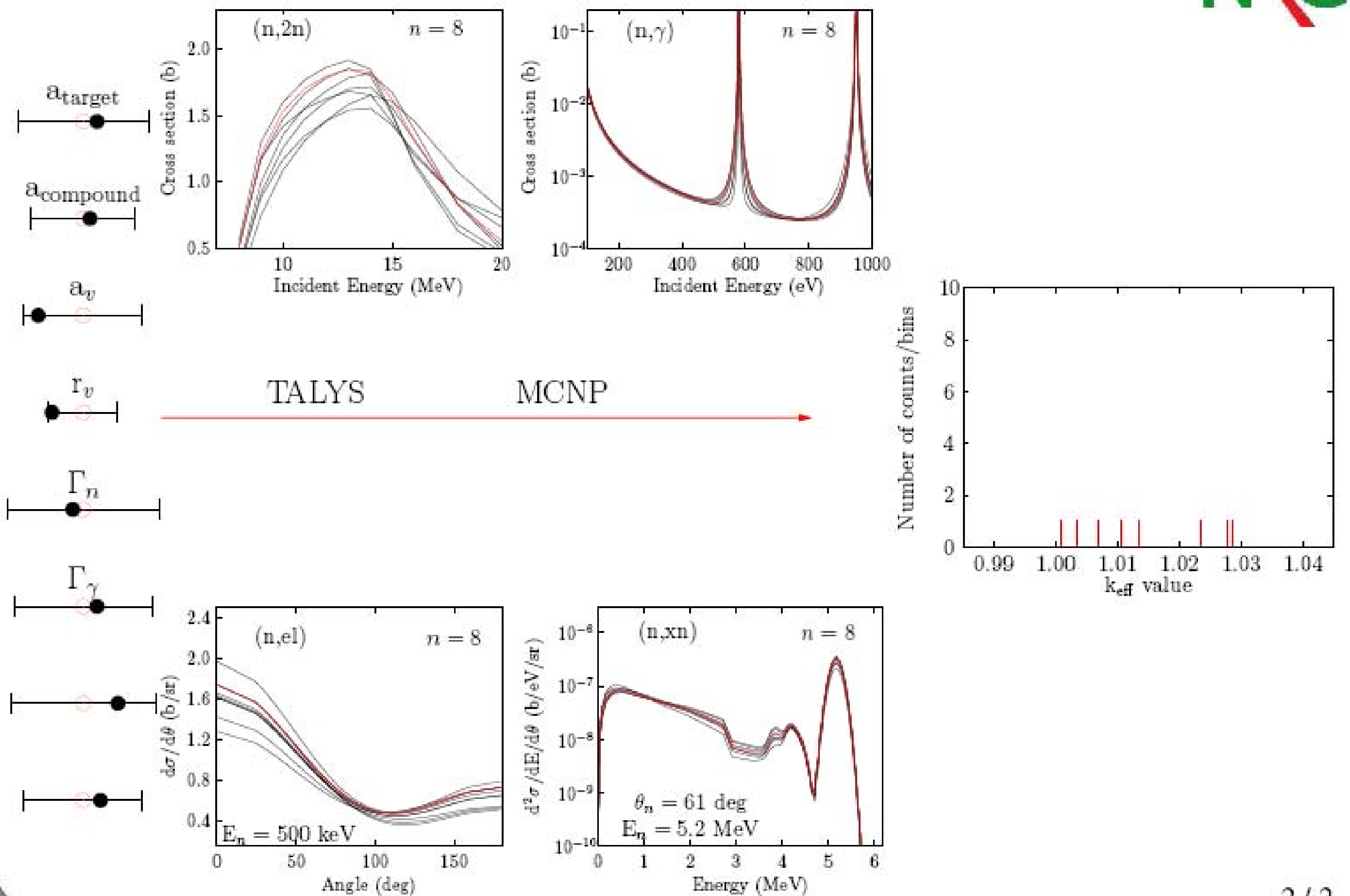

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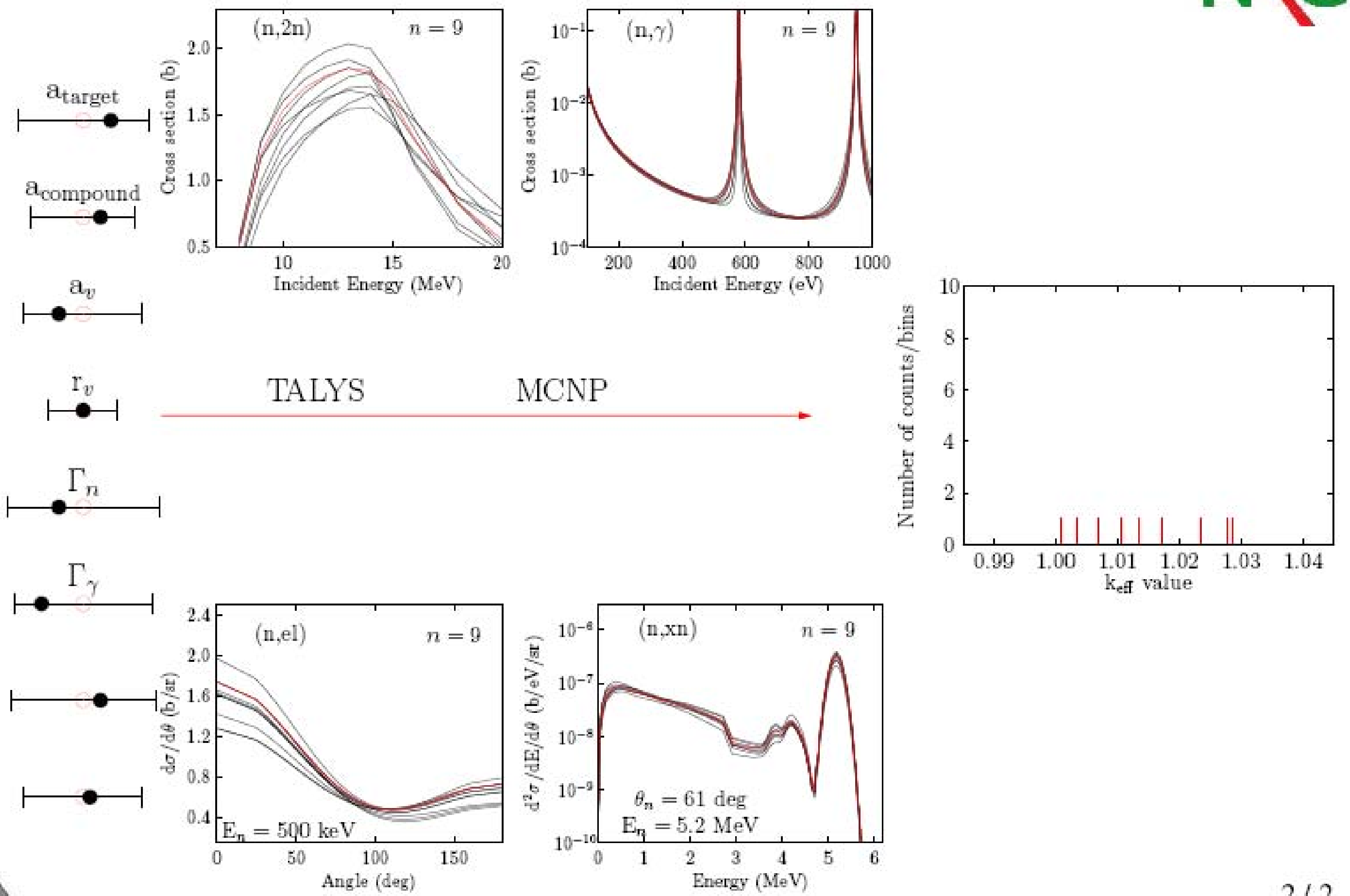

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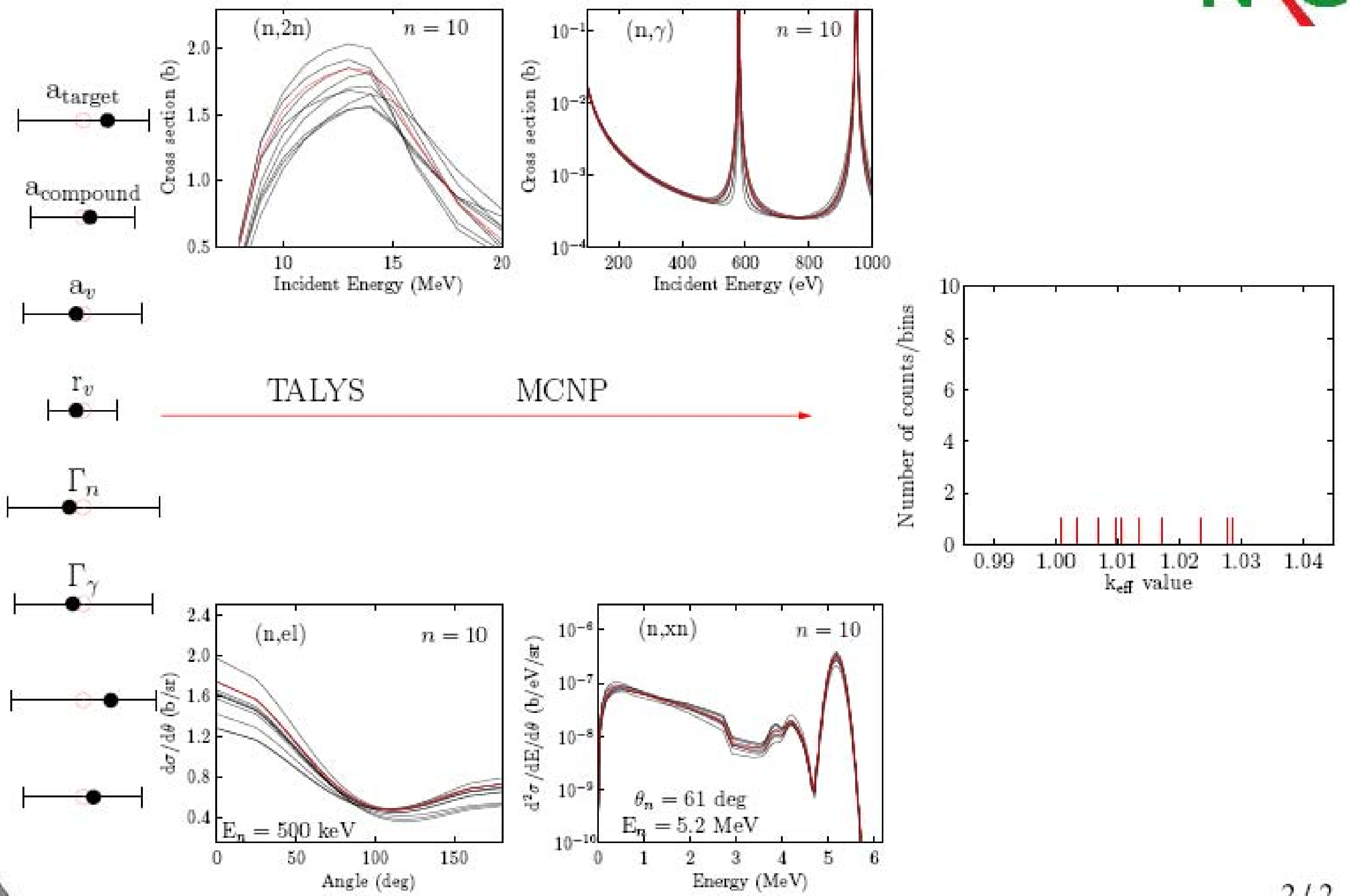

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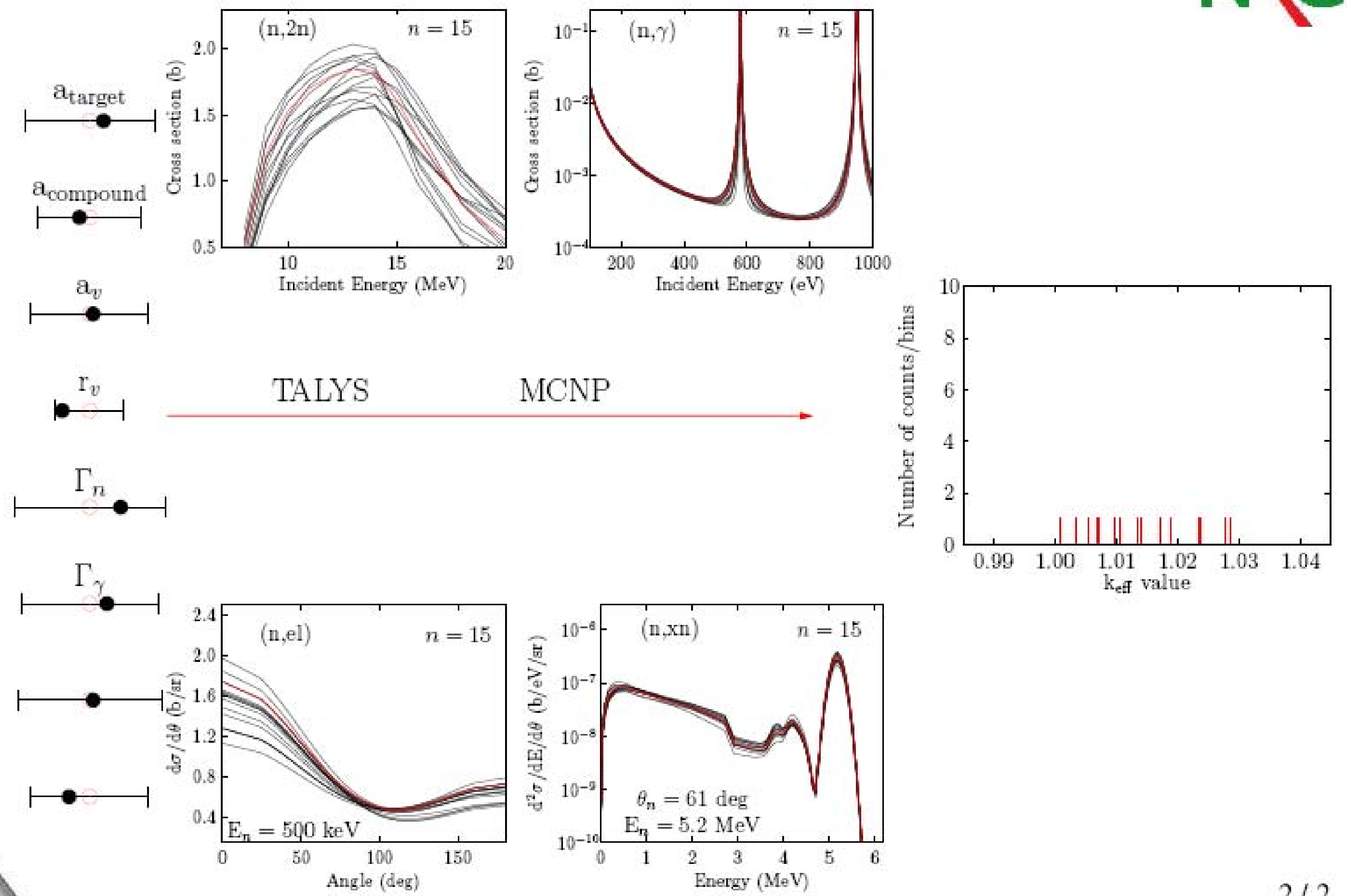

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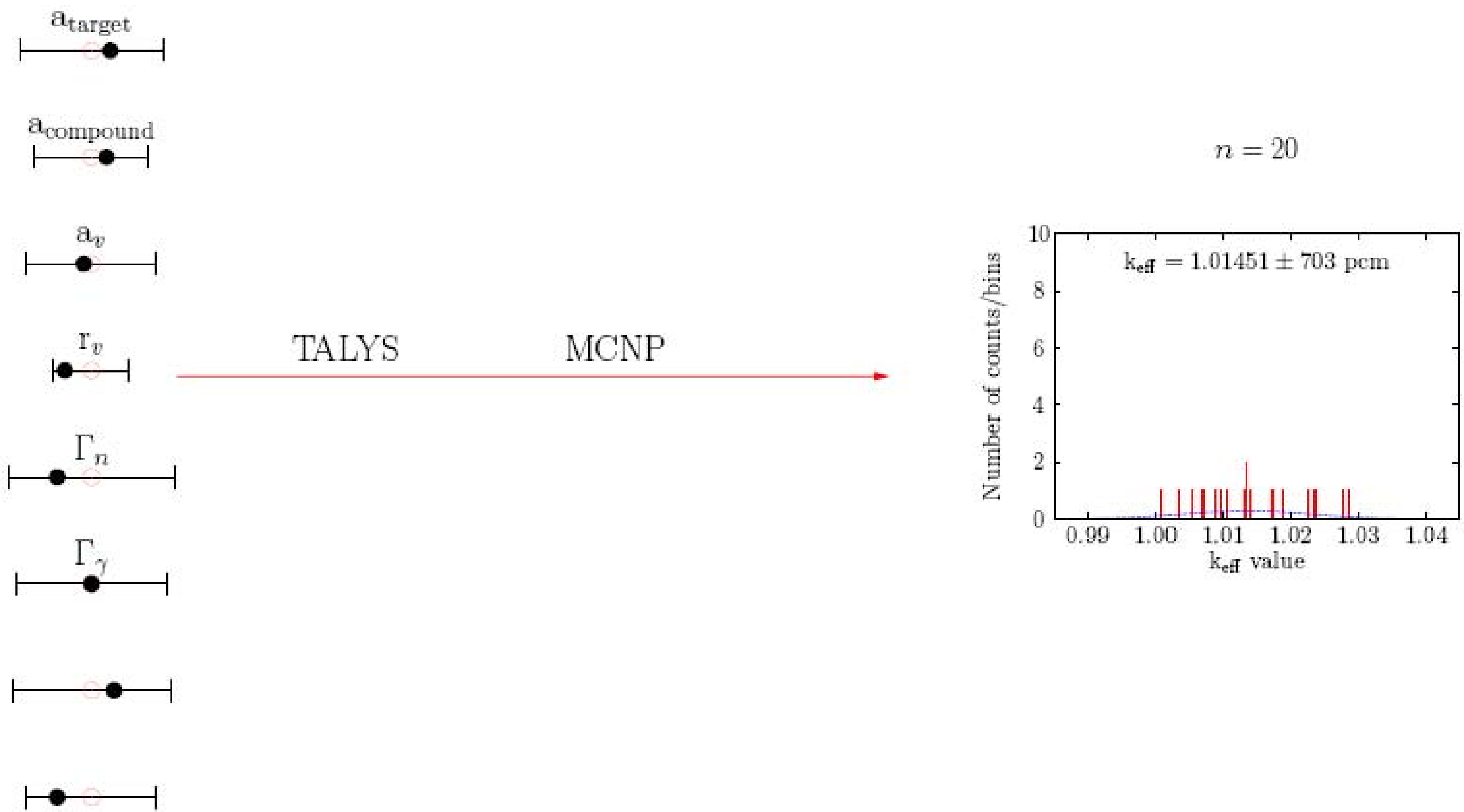

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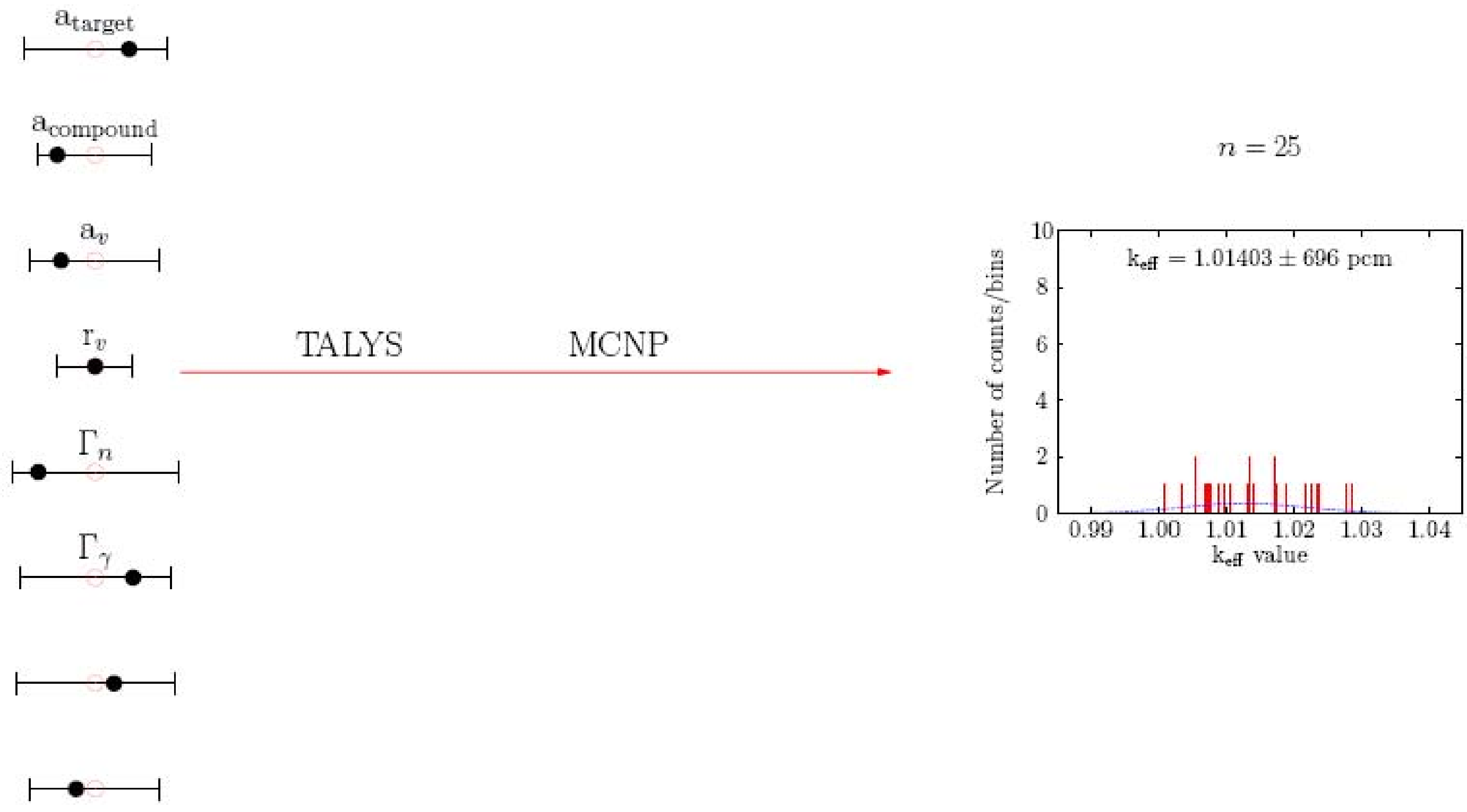

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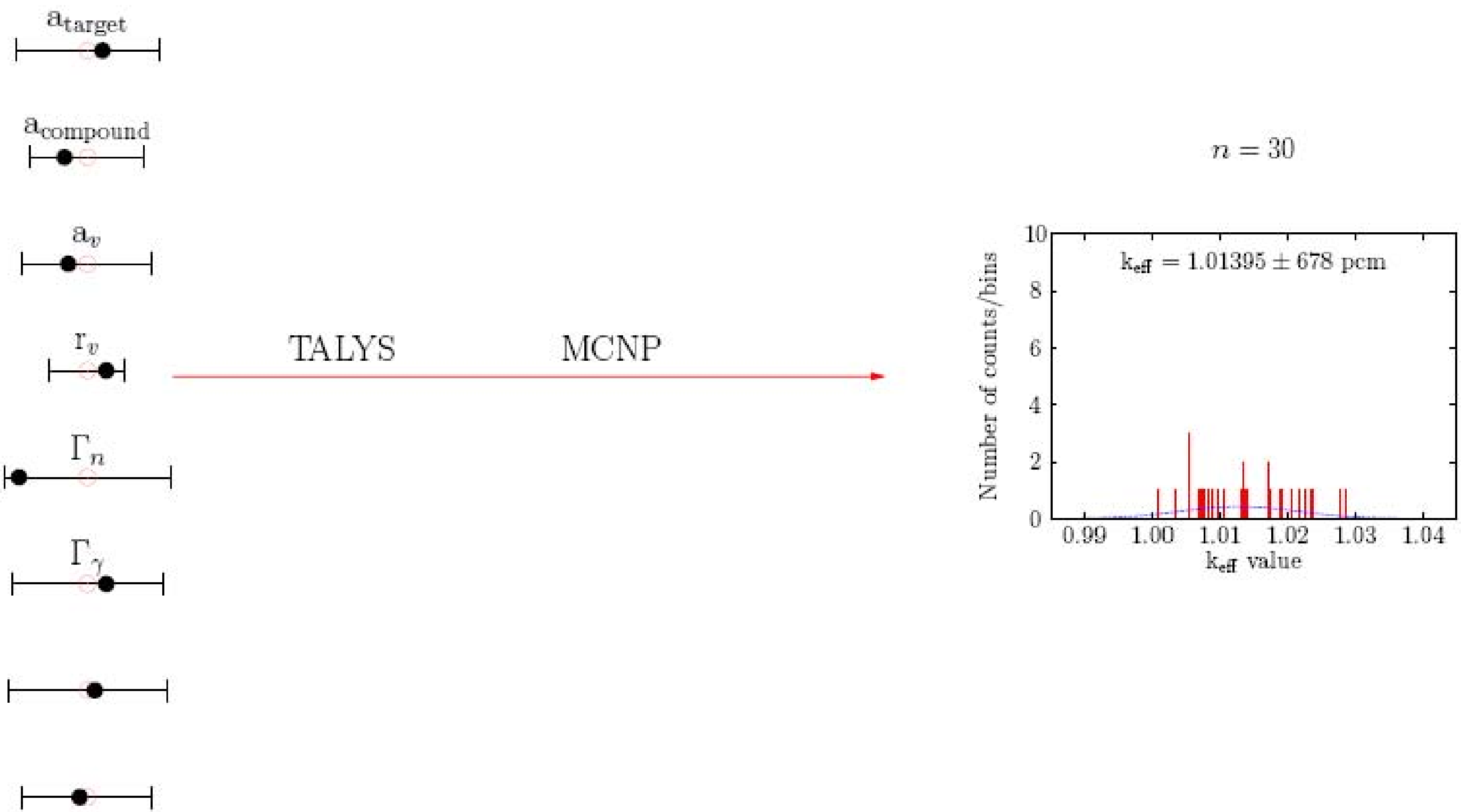

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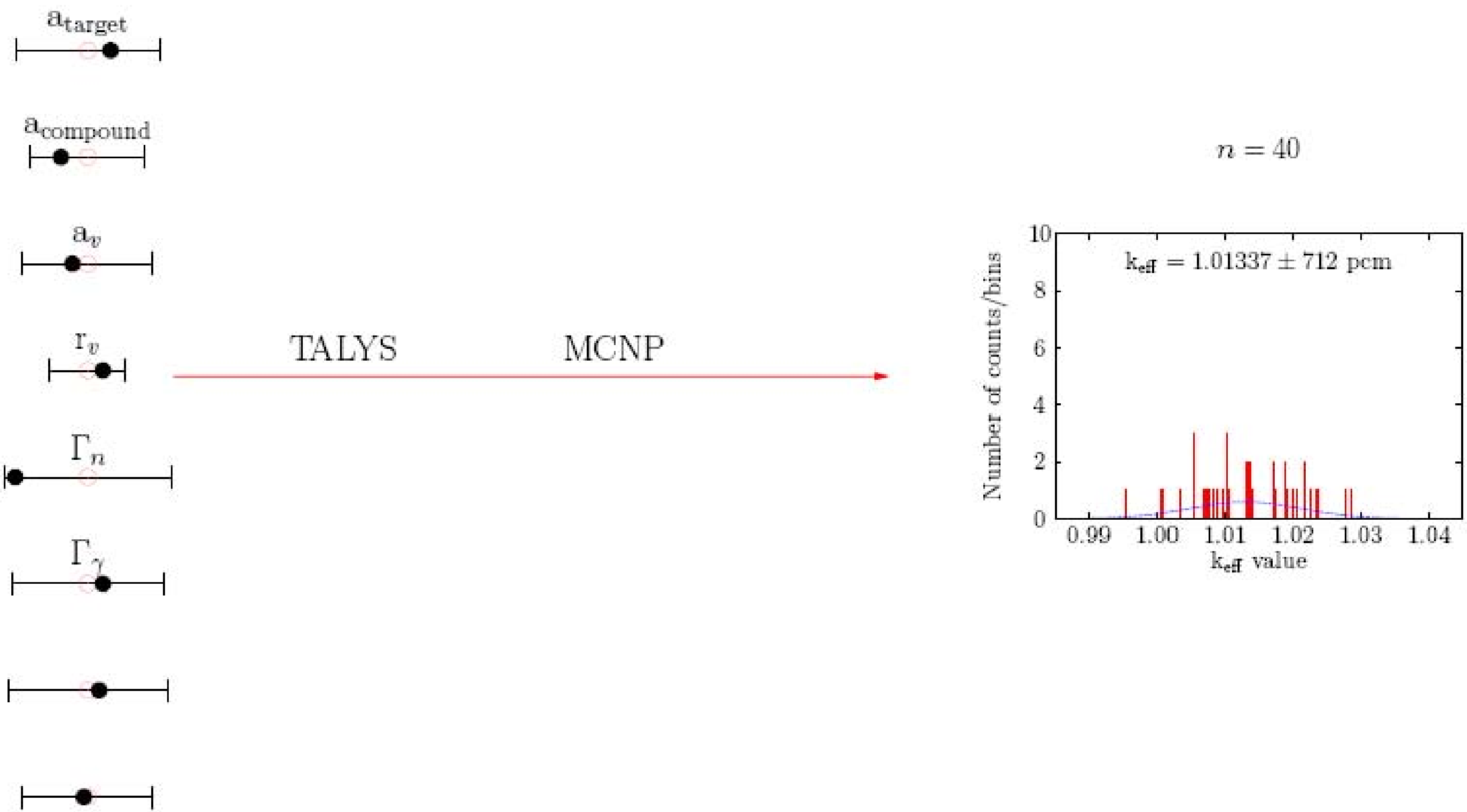

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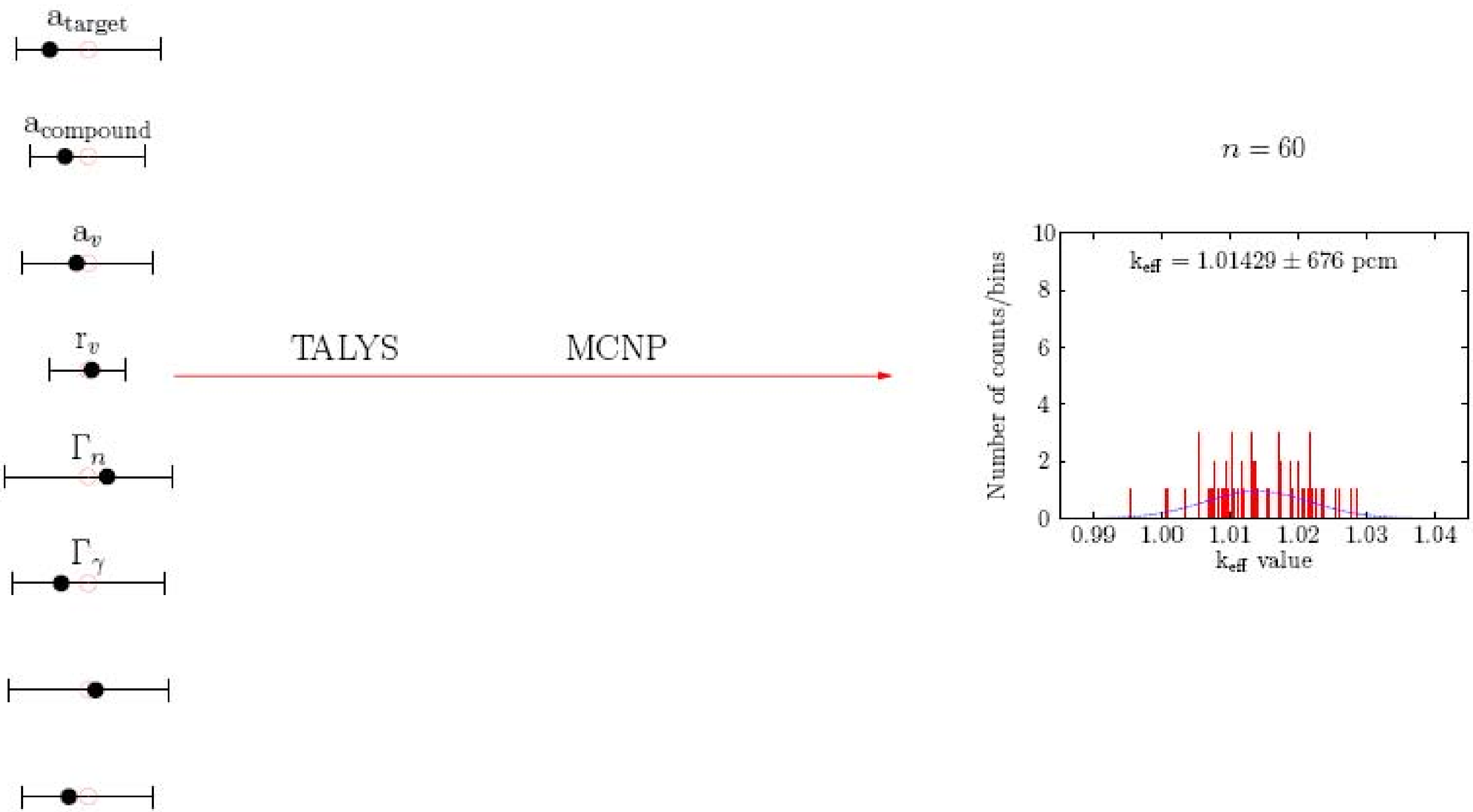

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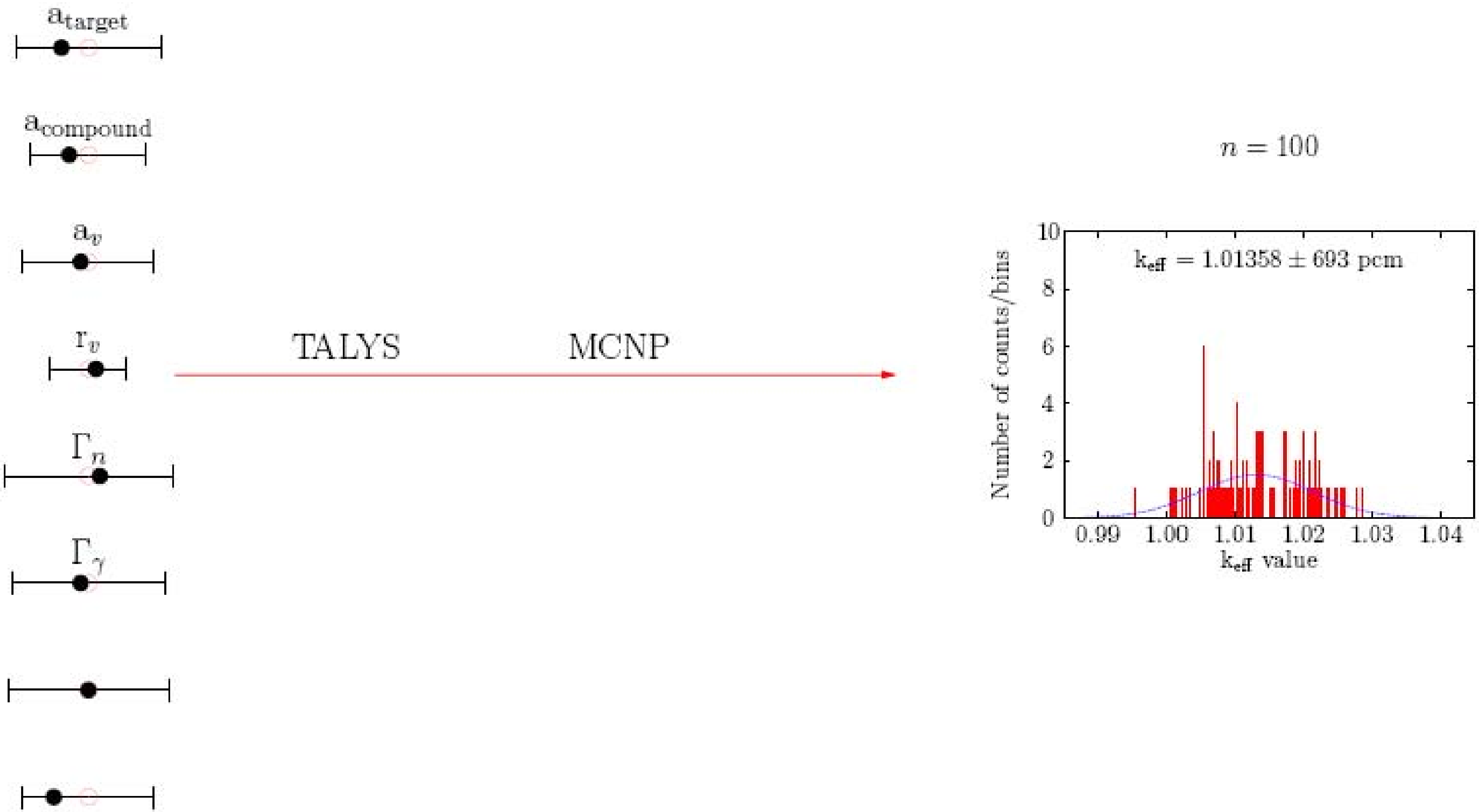

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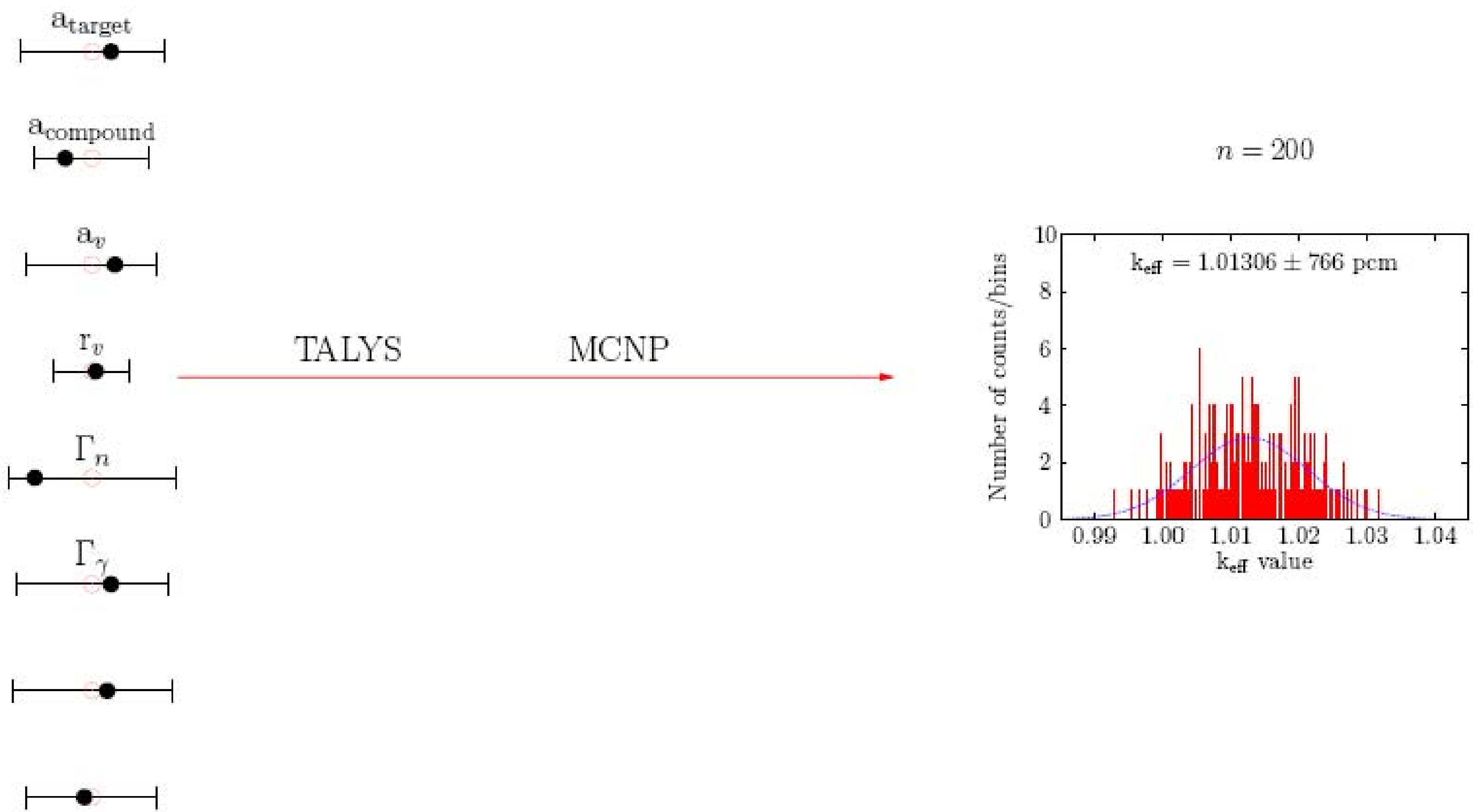

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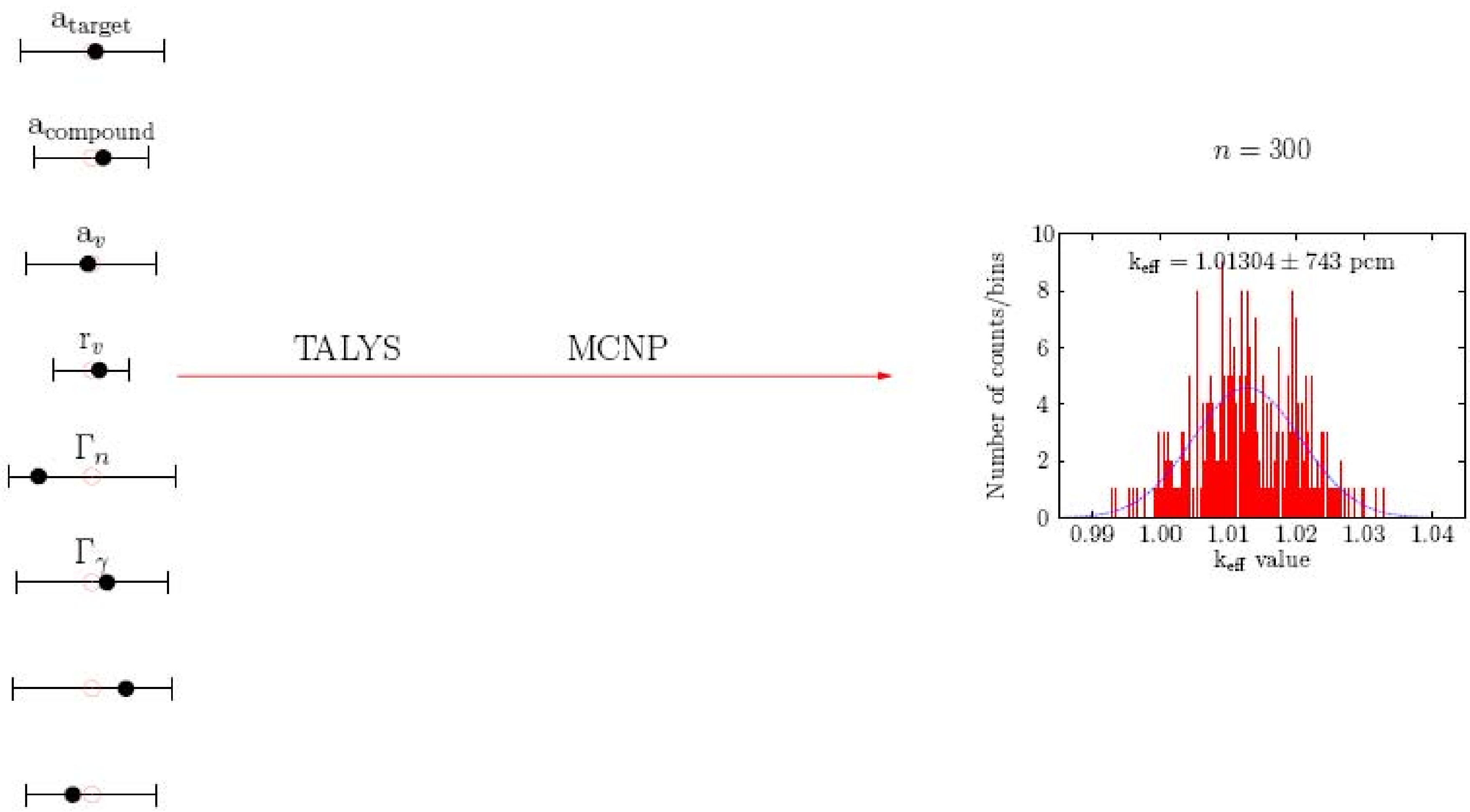

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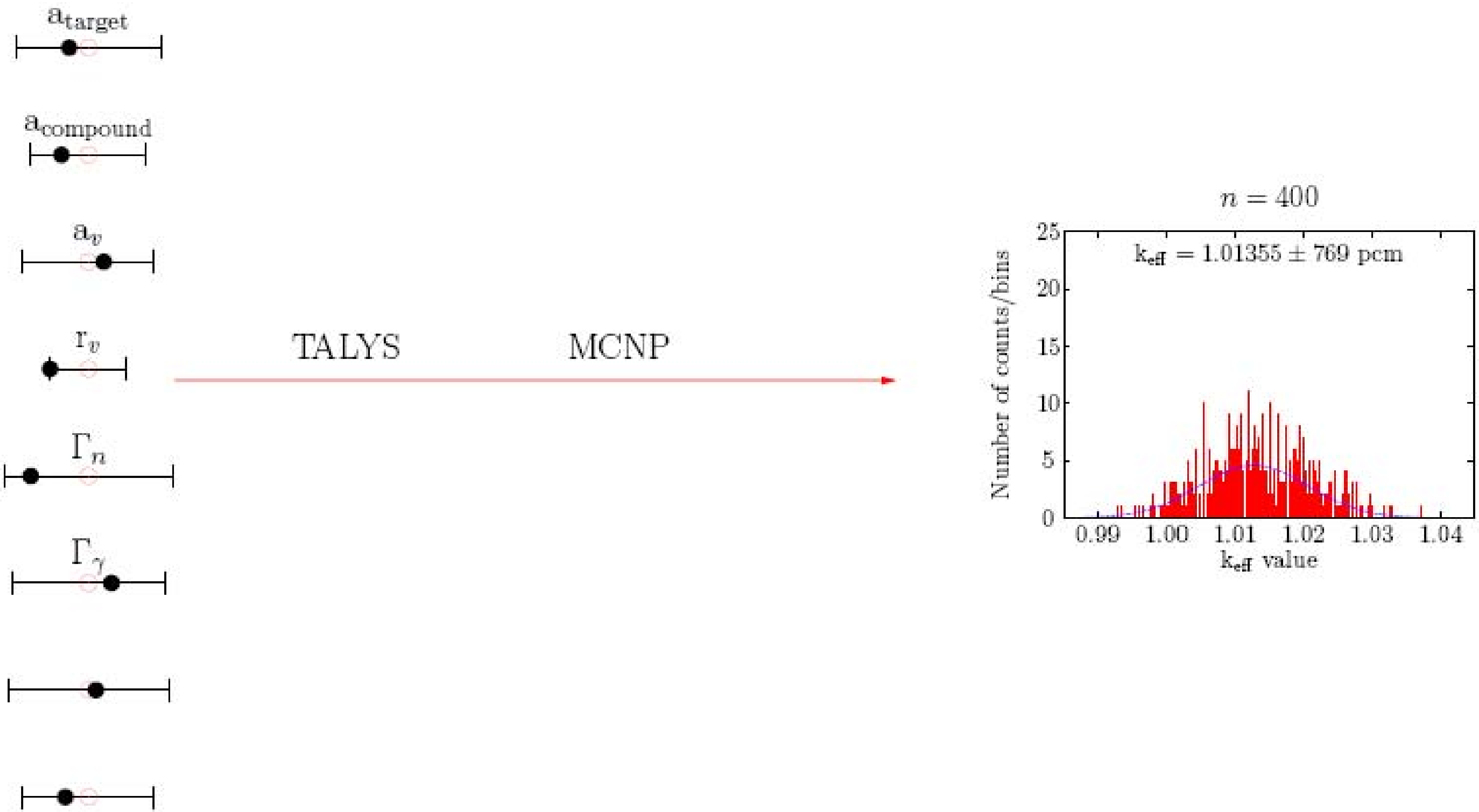

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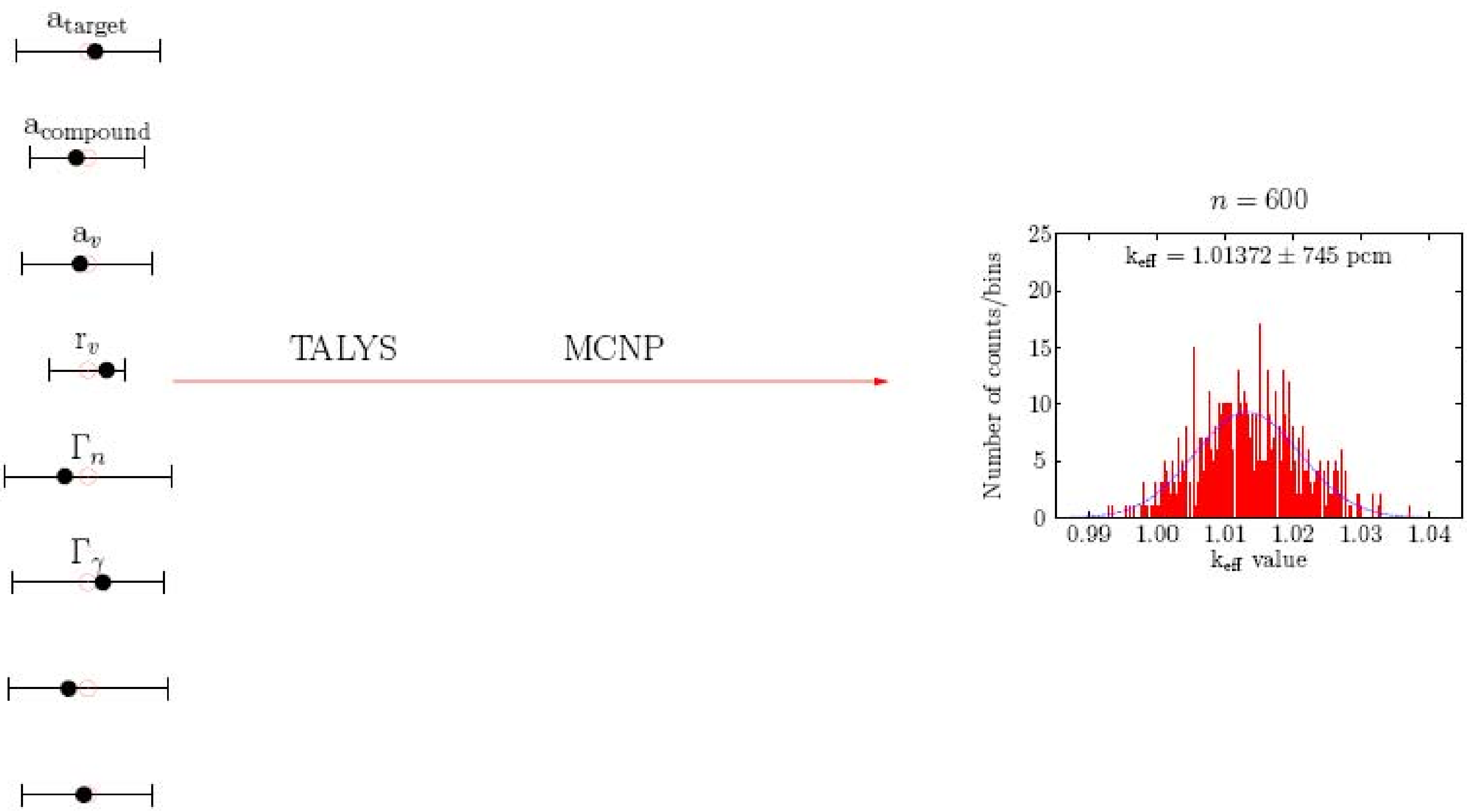

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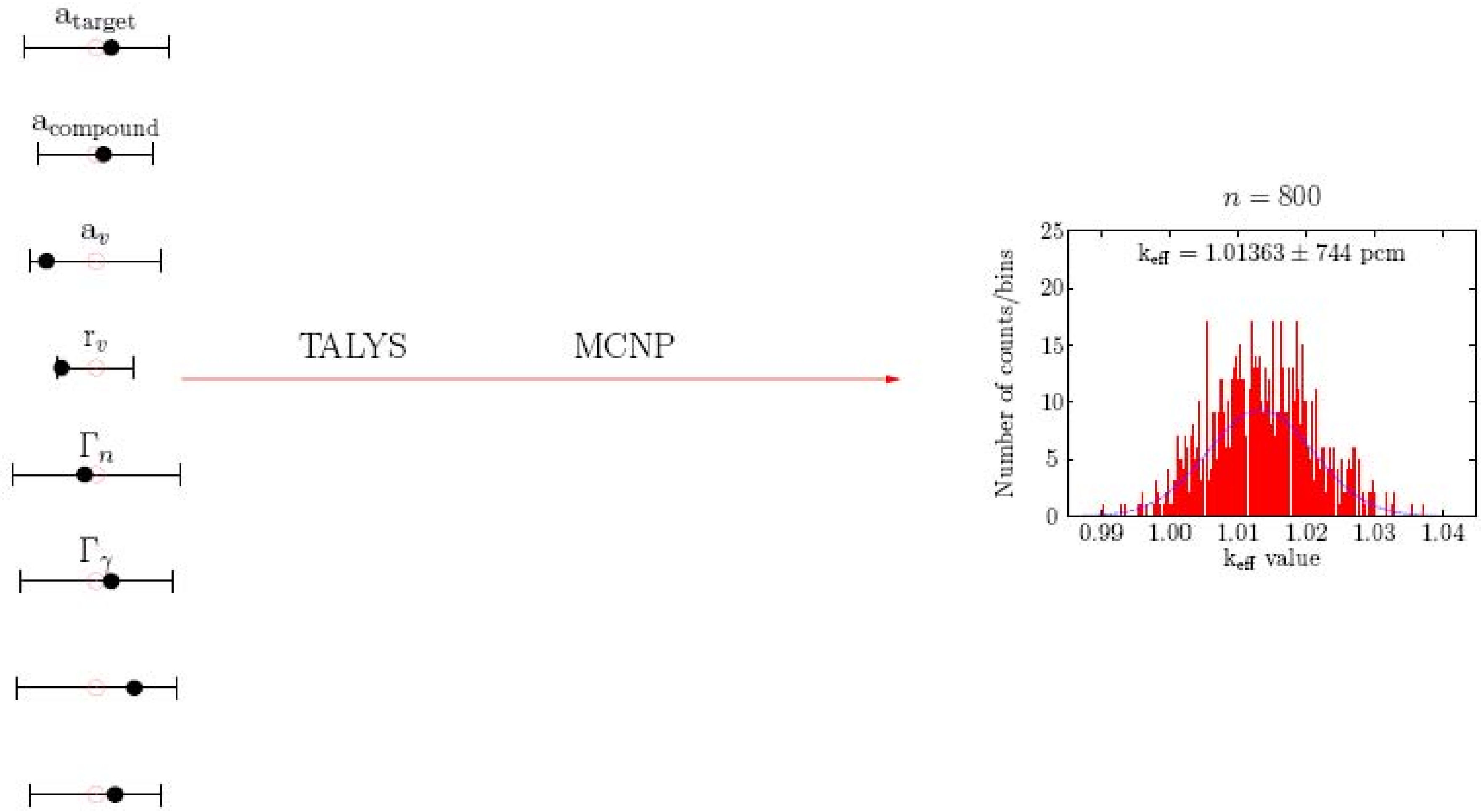

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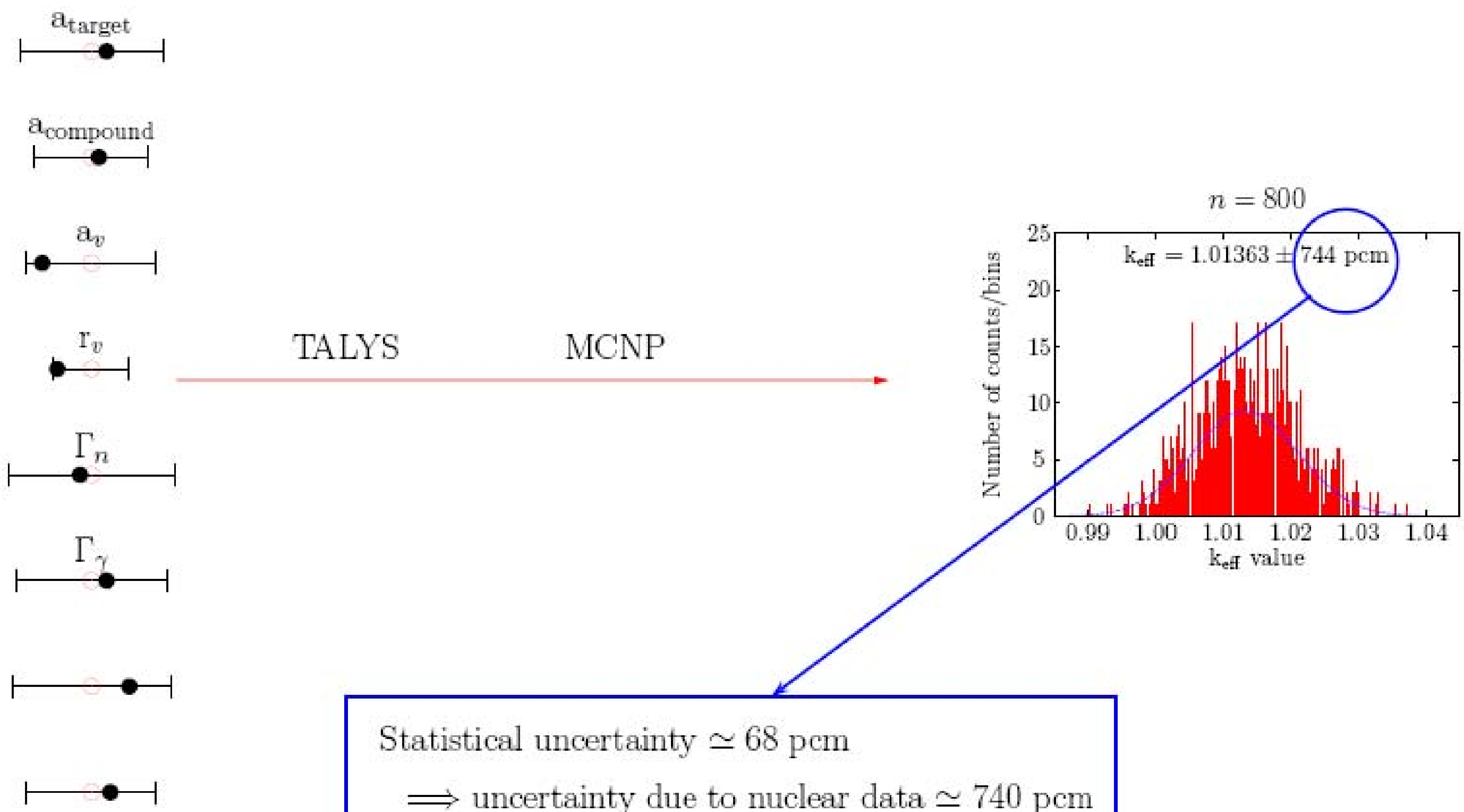
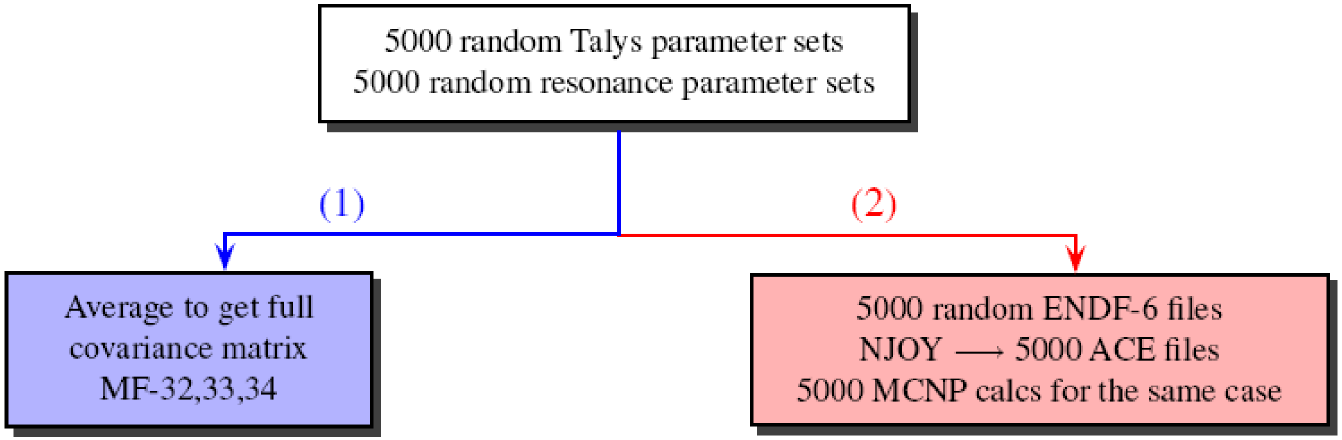


Statistical uncertainty $\simeq$ 68 pcm

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

Covariance versus Total Monte Carlo



Advantages:
- Relatively quick
- Use in sensitivity study
- Easier release (TENDL)

Disadvantages:
- Approximative (cross-correlations)
- No covariance for gamma production, DDX (MF36), etc.
- Requires special processing
- Requires covariance software for application codes

Advantages:
- Exact
- Requires only “main” software

Disadvantages:
- (Computer) time consuming
- Backward (sensitivity) route not obvious

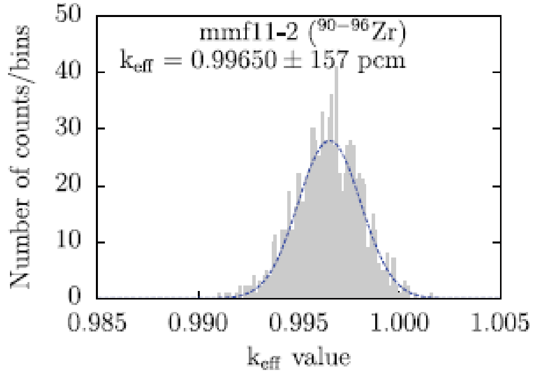
Application: criticality benchmarks

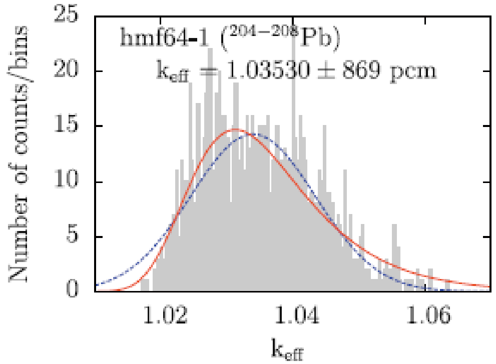
Total of 60000 random ENDF-6 files

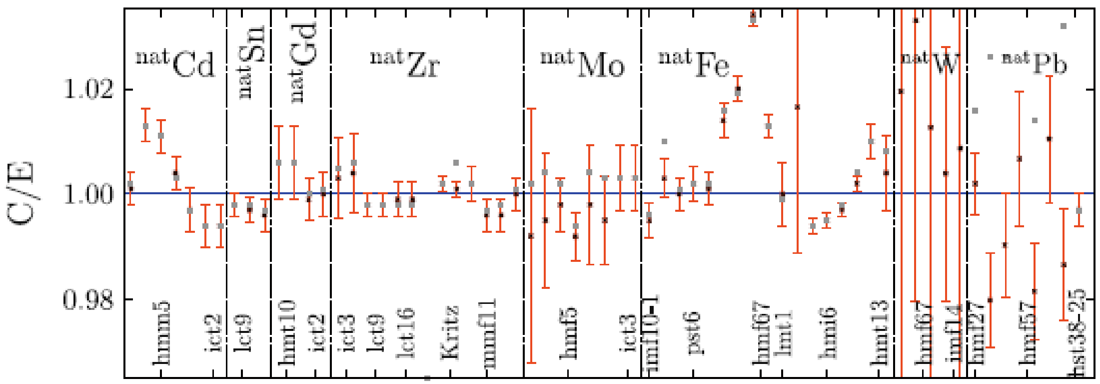
Sometimes deviation from Gaussian shape

Rochman, Koning, van der Marck
Ann Nuc En 36, 810 (2009)

Yields uncertainties on benchmarks

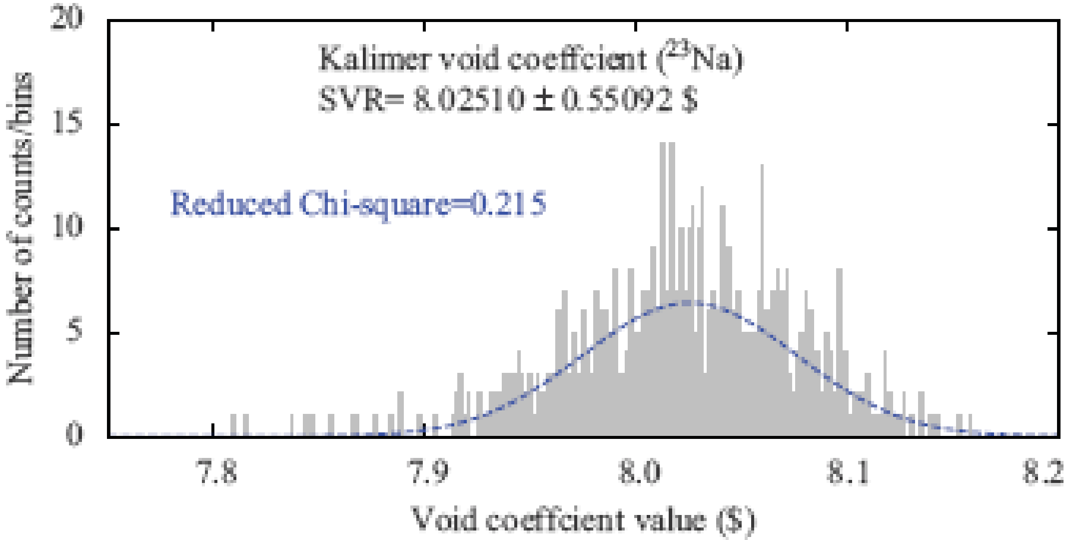




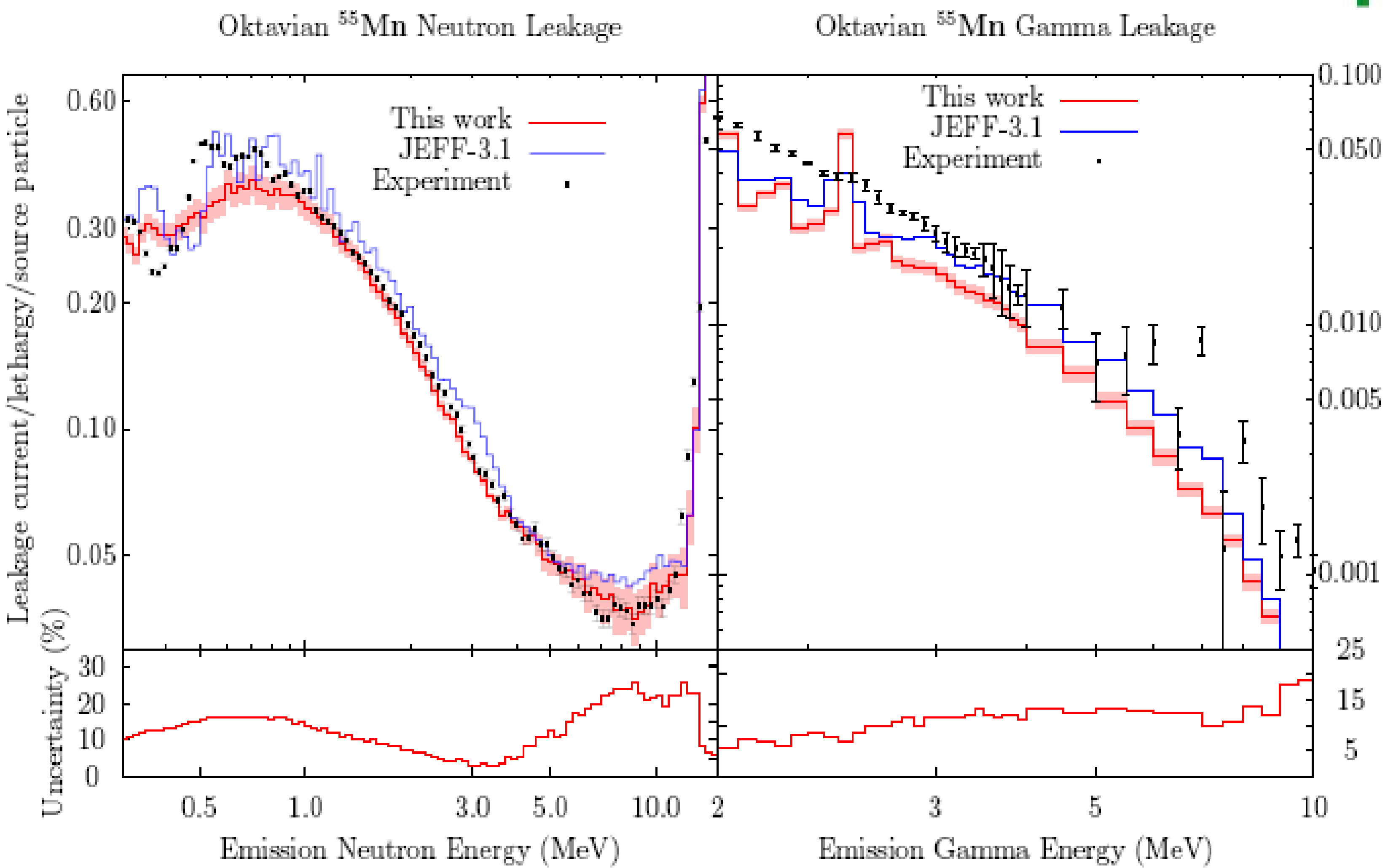


Application: SFR void coefficient

- KALIMER-600 Sodium Fast Reactor (Korea)
- Total Monte Carlo with MCNP
- Uncertainties due to Na: D. Rochman et al NIM A612, 374 (2010)
- Extension to SFR burn-up underway

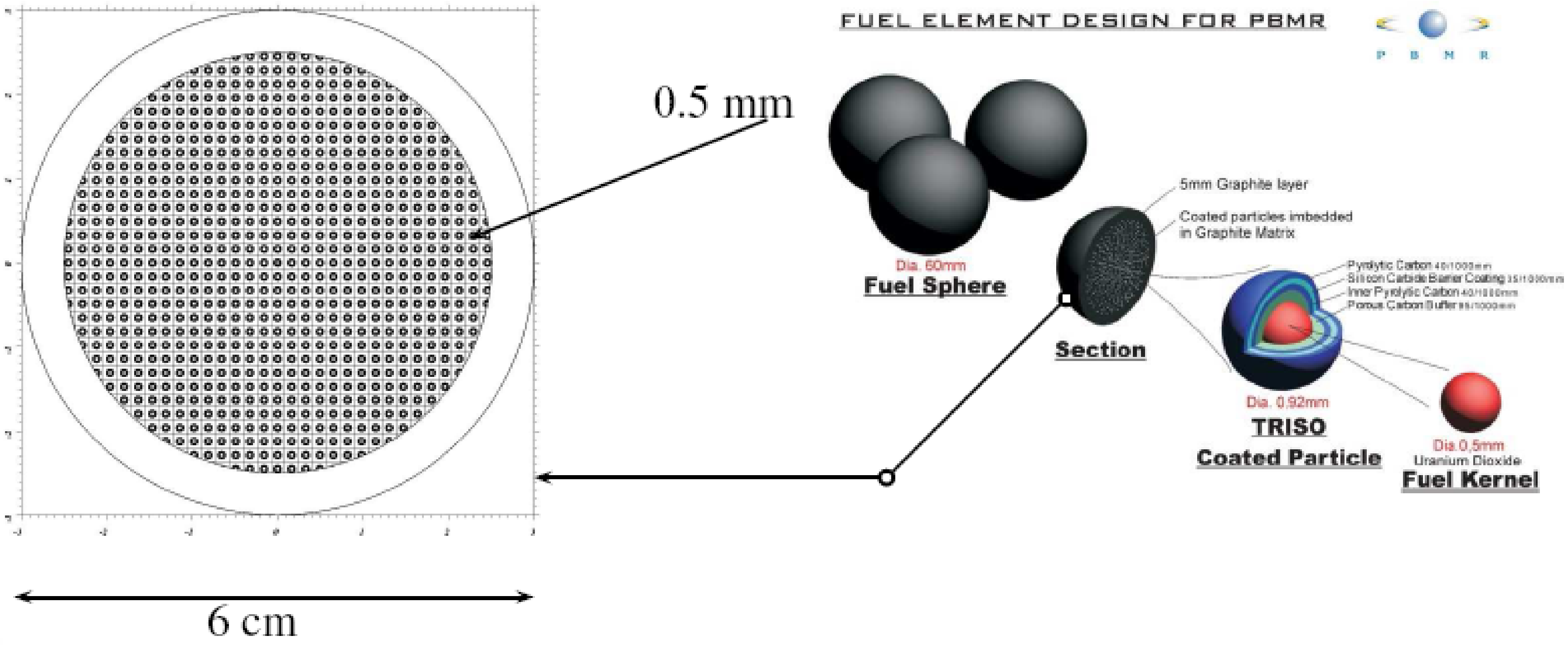


Application for Mn Oktavian benchmark



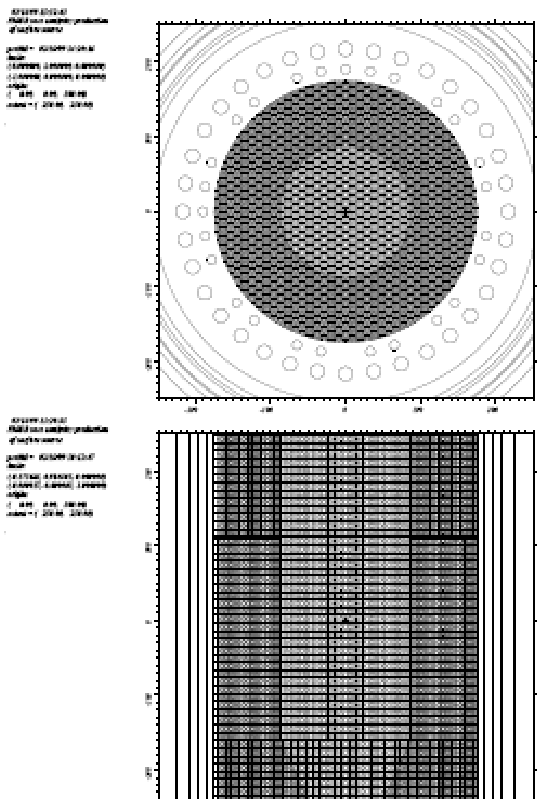
Application: Pebble Bed Modular Reactor (PBMR)

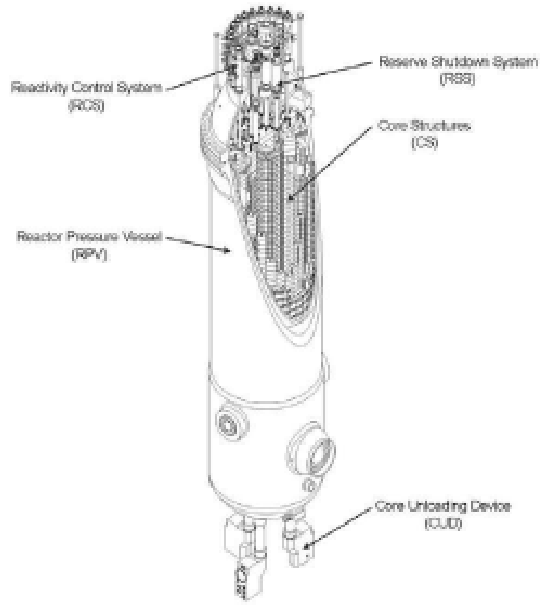
- Model of a fuel pebble
- Fuel particles, surrounded by coating layers, explicitely modelled
- Regular rectangular lattice of fuel particles



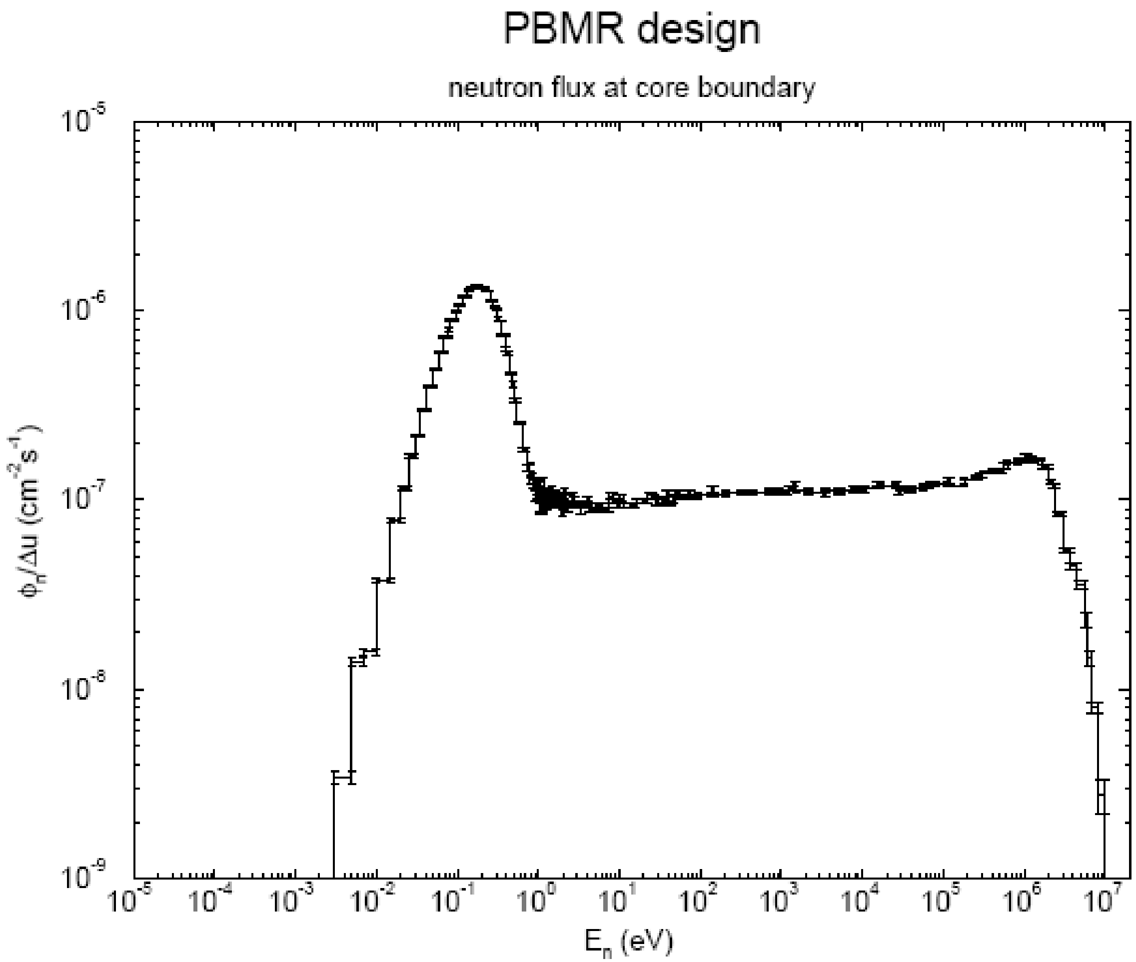
Application: Pebble Bed Modular Reactor (PBMR)

- Hexagonal close packed lattice
- Moderator region consists of homogeneous moderator pebbles as the fuel, reflectors and shields as defined by ESKOM





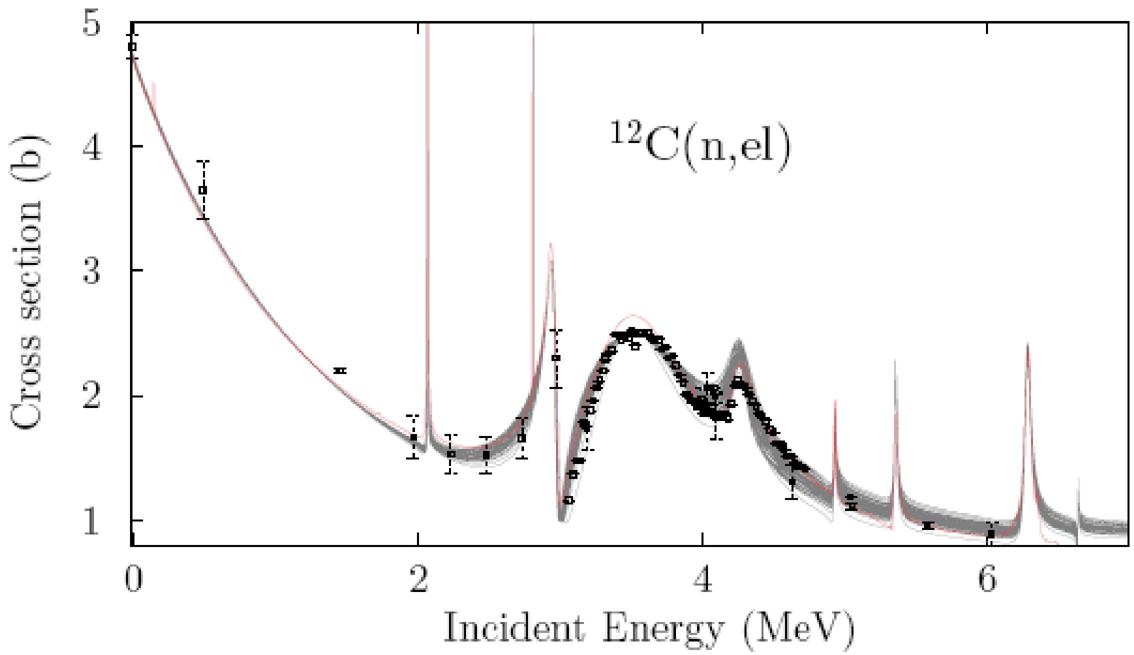
PBMR: neutron flux spectrum



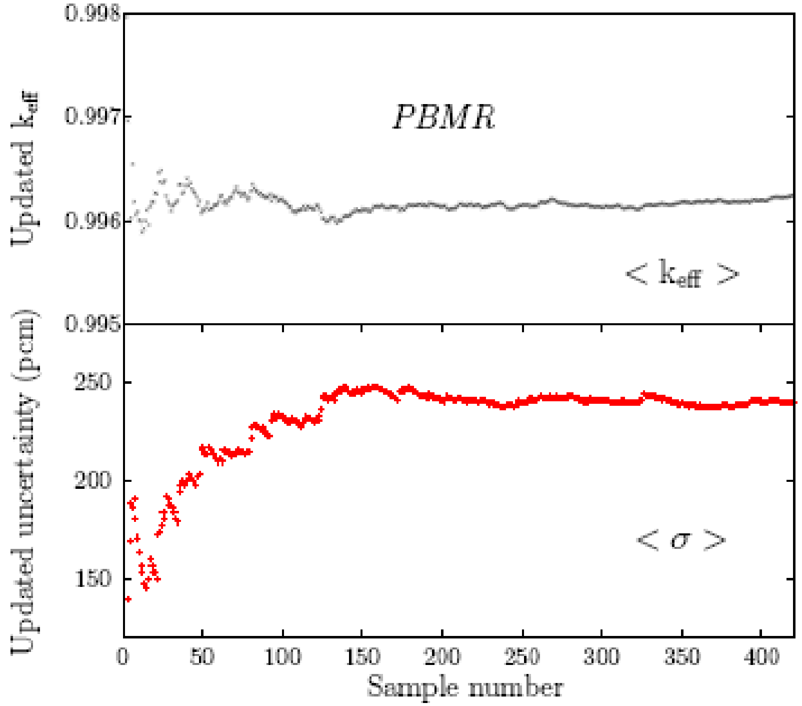
Neutron flux spectrum at the radial core boundary (Almost no neutron above few MeV)

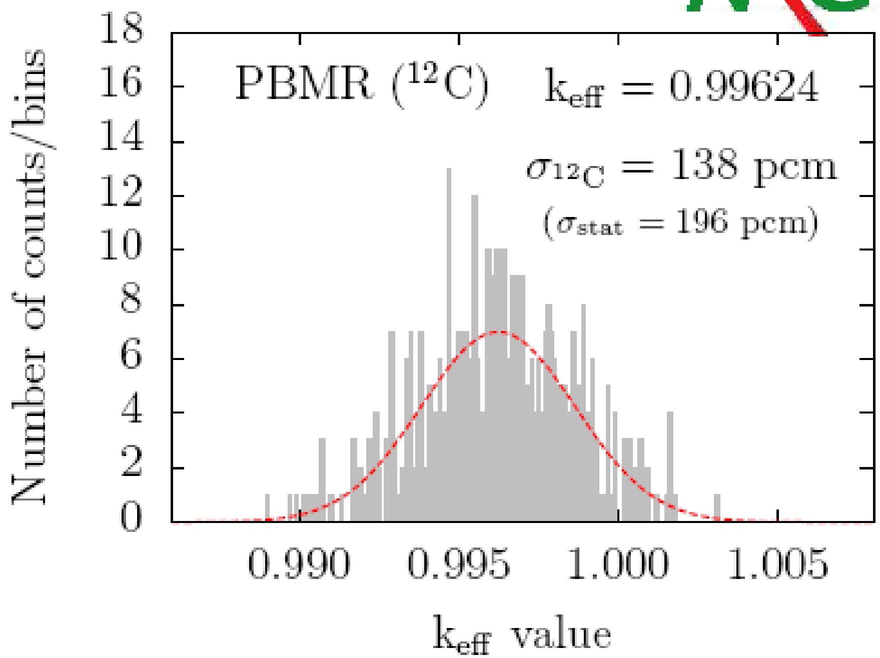
PBMR: C-12 nuclear data

- For neutron energy lower than few MeV: only elastic and capture cross sections
- JEFF-3.1: σ_{th} (n,el)$= 4.746 \pm 0.002$b and σ_{th} (n,γ)$= 3.53 \pm 0.07$mb
- All (n,el), (n,γ), angular distribution and emission spectra randomly varied



PBMR: Results





- Convergence achieved after $\simeq$ 350 runs (10 days of 15 CPU)
- More runs would be suitable
- Effect of other isotopes (^{13}C, Si, fission products and of course actinides)

TMC: Other possibilities

- Random thermal scattering data libraries (?)
- Random decay data libraries
- Random fission yield libraries
- Normalization to experimental data or other nuclear data libraries at the basic input level (in progress)
- Optimization to integral benchmarks using e.g. simulated annealing (“search for the best random file”)

Library	Normalized χ^2_N					
	Global	LEU	HEU	^{239}Pu	Other	^{233}U
	686	285	200	117	67	17
ENDF/B-VII.0	1.00	1.00	1.00	1.00	1.00	1.00
ENDF/B-VI.8	1.19	1.68	1.24	0.88	1.12	2.52
JEFF-3.1	1.13	0.91	1.39	0.85	1.04	1.68
JENDL-3.3	1.30	1.04	1.42	1.39	1.12	0.42
TENDL-2009β	0.98	1.05	0.97	0.93	1.01	0.90

Conclusions

Nuclear model parameter uncertainties can be propagated to uncertainties of cross sections, angular distributions, spectra, etc. using a Monte Carlo approach:

- TALYS is robust and fast enough for this
- Global uncertainties are available for all TALYS parameters. This gives rather realistic cross section uncertainties already. If experimental data is available, parameter uncertainties will get smaller.
- Next question: how to take into account experimental uncertainties in a coherent approach? (Later this week: see and hear Roberto Capote)

Conclusions

The lifetime of the Nuclear Data Cycle (from basic data to applications and back) can be strongly reduced, even using existing formats and tools.

The secret:

- Make everything reproducible from the start. Ingredients:
  - Selected experimental data from EXFOR (if available)
  - TALYS input parameters + uncertainties (or default)
  - Resonance parameters + uncertainties (if available)
  - Nuclide specific scripts (if needed)
- After some serious software development you can reproduce everything from that
- The first two applications
  - Talys Evaluated Nuclear Data Library (TENDL)
  - Total Monte Carlo uncertainty propagation

Conclusions

The system is in place, from now on the main challenges are at the beginning of the cycle, e.g.:

- Better evaluations per nuclide
- Merge experimental + theoretical uncertainty methods ("Unified Monte Carlo")

Of course, this approach does not take away the need for progress in measurements, theory development, ENDF formatting, processing and validation,

but any progress will have impact directly through the entire chain, and for all nuclides (reproducibility!)

Acknowledgements

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IAEA: Roberto Capote

JUKO research: Jura Kopecky

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