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D. Rochman

Nuclear data uncertainty propagation

Part 1: introduction and TMC.

EXTEND summer school, Uppsala University, Sweden, September 1st, 2016

Zertifiziertes Managementsystem STARS ISO 9001

Summary

- What are nuclear data (*Part 1*)
- Are they important ? (*Part 1*)
- How can they be produced for application (*Part 1*)?
- ND Uncertainties and their propagation (*Part 1*)
- TMC (*Part 1*)

- TMC + adjustment (*Part 2*)

- Applications to energy systems (*Part 3*)

All slides can be found here: https://tendl.web.psi.ch/bib_rochman/presentation.html

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Some general facts

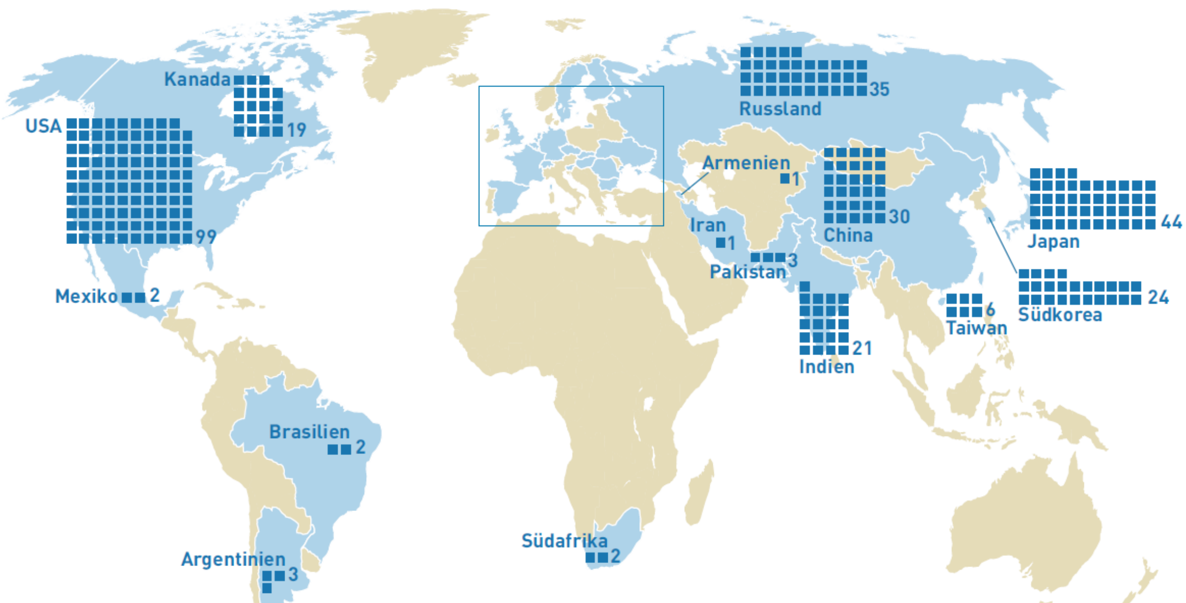
Kernkraftwerke weltweit

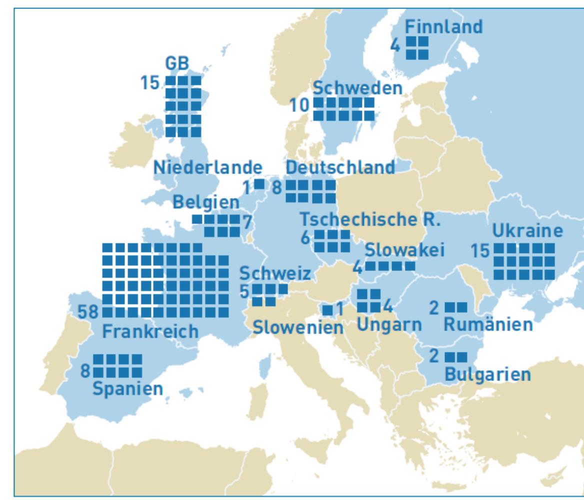
Les centrales nucléaires du monde

Stand 31.12.2015* / Etat au 31 décembre 2015*

Ganze Welt 442 383 500 MW 11 %

Monde entier





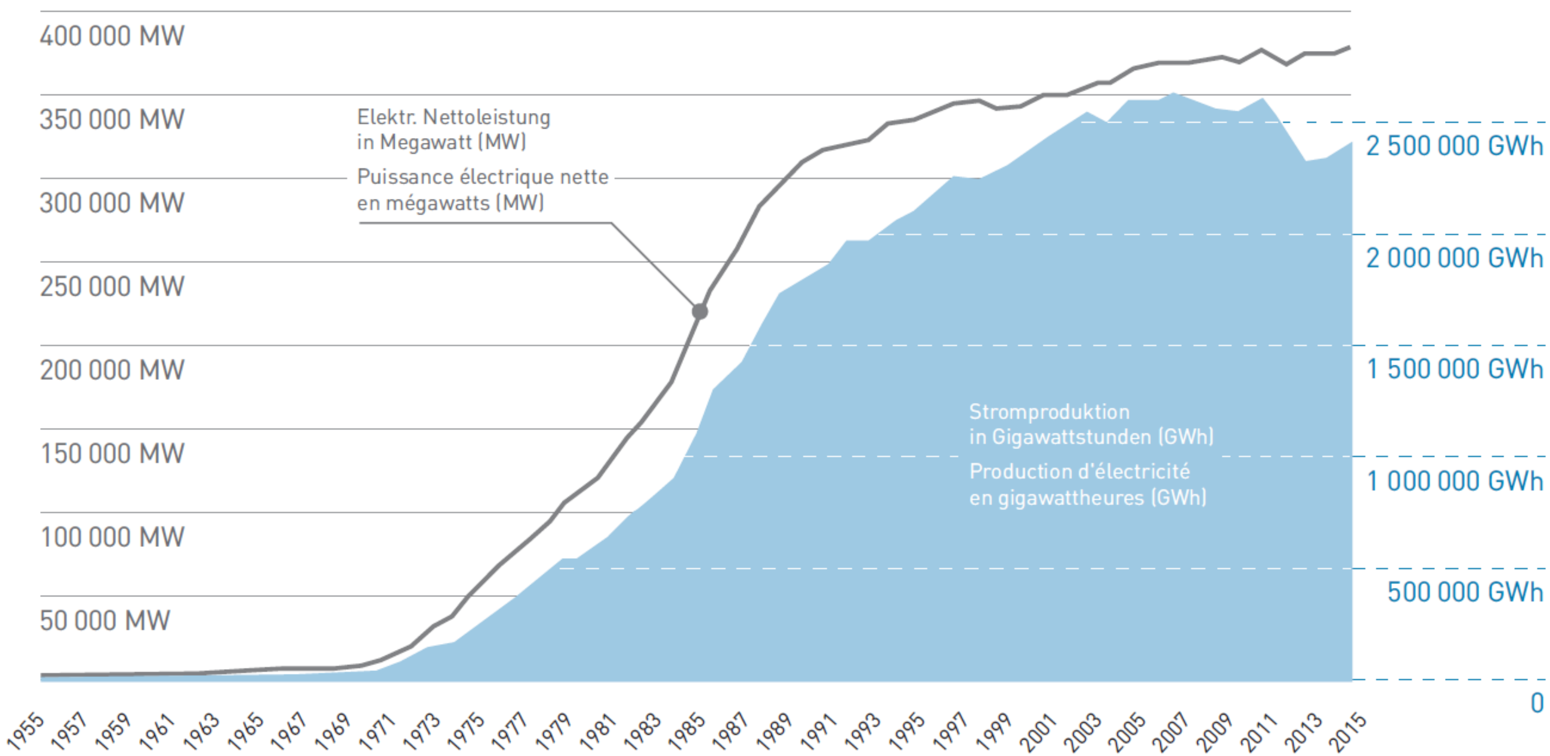
* Aktuelle Daten zu den Kernkraftwerken und Lagern der Welt auf: www.nuclearplanet.ch

Les données relatives aux centrales nucléaires et aux dépôts de déchets radioactifs du monde entier sont mises à jour sur:

Some general facts

Leistung und Stromproduktion
der Kernkraftwerke weltweit von 1955 bis 2015

Puissance et production d'électricité
des centrales nucléaires dans le monde de 1955 à 2015



What is “nuclear data” ?

The term “Nuclear data” can have different meaning:

- Old and dusty books, constants, mature field, code inputs, parameters
- Listing, Schrodinger equation, unexciting…
- But it is not !

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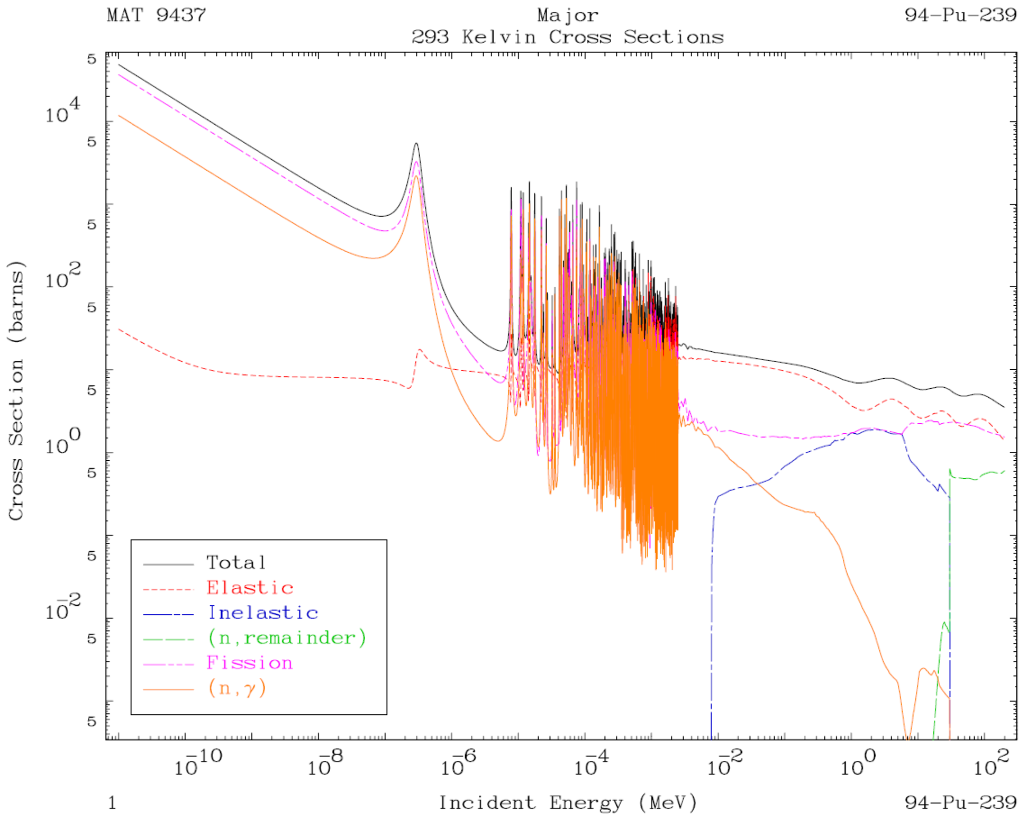
What are nuclear data in this presentation ?

- From ^{1}H to ^{280}Ds,
- From 0 to 20(0) MeV neutron induced,
- Cross sections, particle emission,
- Angular and energy distributions
- Decay data (half-lives, gamma-ray,…), fission yields, neutron yields,
- And uncertainties



- All these data are nicely condensed in text files in ENDF-6 format (80 columns)

Are nuclear data important ?

In energy production, better nuclear data can help for:

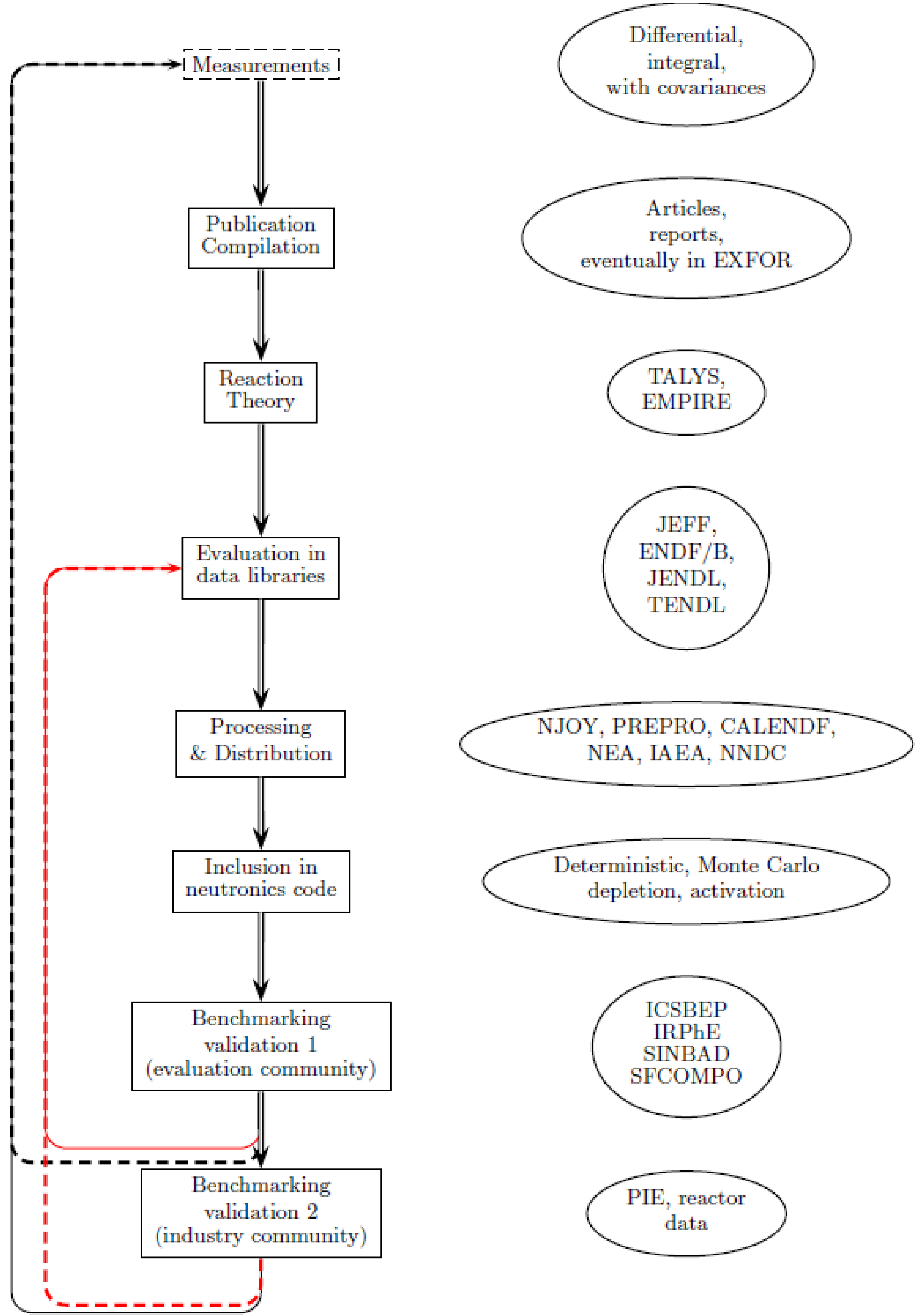
- Fuel storage and processing,
- Life-time extension,
- Outside usual reactor operations,
- Dosimetry,
- Higher fuel burn-up,
- cost reduction in design of new systems,
- Isotope production,
- Shielding (people safety),
- Future systems,

Dry fuel storage, Zwilag, Switzerland

Better nuclear data have a limited effect on:

- Current reactor operation,
- Current reactor safety,
- Accident simulation,
- Proliferation,
- Chernobyl, TMI, Fukushima and other accident.

Nuclear data life cycle



How to produce nuclear data ?

Independently of the quality of the data, there are 2 ways to produce them:

First solution: manual production

- Widely used for decades up to 2100,
- Concerns all major libraries,
- Questionable QA practices (≠ than the industry standards),
- Has produced very good data,
- We know less and less why.

Second solution: “computer-assisted” production

- One word: “reproducibility”,
- Concerns only one library: TENDL
- Much better QA,
- Spent your time on the physics (evaluation), not on the format

The world perception is changing and the second solution might spread around.
See TALYS lab for practical exercises.

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How to use nuclear data ?

In general, nuclear data files/evaluations are used by simulation codes:

Neutron transport,

- Monte Carlo: MCNP, SERPENT, TRIPOLI, MONK…
- Fuel assembly (lattice) deterministic: SCALE, DRAGON, CASMO, APPOLO…
- Full core deterministic: SCALE, PANTHER, SIMULATE, DARWIN…
- Transient: S3K,RELAP…

Isotope inventory, radioprotection

- Depletion: FISPACT, ORIGEN, CASMO, SERPENT,…
- Fuel inventory/decay heat: SNF, FISPACT,…

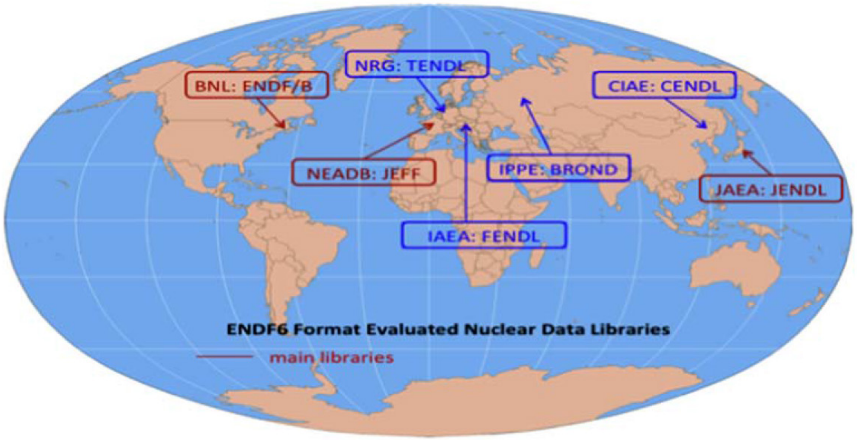
But prior to use them, some processing of the nuclear data is needed:

- NJOY (USA LANL),
- CALENDF (France CEA),
- PREPRO (USA LLNL),
- AMPX, PUFF (USA ORNL),
- WIMS (UK), and many other.

Nuclear data libraries

Historically, there exists today many nuclear data libraries:

- <u>General purpose</u>
  - JEFF, mostly towards reactor applications
  - JENDL, mostly towards reactor applications
  - ENDF/B, mostly towards reactor applications
  - TENDL
  - BROND, mostly towards reactor applications
  - CENDL, mostly towards reactor applications
- <u>For fusion application</u>
  - FENDL
  - TENDL
- <u>For dosimetry</u>
  - IRDFF
  - TENDL
- <u>Plus all derived libraries</u>



Processing nuclear data libraries

This is a very specific task, sometimes secretive, sometimes with specific parameters

Most simple processing: nothing done

- Fission yields, decay data,
- Libraries are read as they are by simulation codes

More sophisticated:

- For Monte Carlo transport calculation (MCNP, SERPENT)
- Usually performed with NJOY
- Can take hours: pointwise, groupwise data, Doppler broadening, reconstruction of emission spectra…

One step further:

- For Deterministic transport calculation,
- Performed with many processing codes,
- As for Monte Carlo, + self-shielding factors,
- Not always in the open literature (expert knowledge).

Nuclear data uncertainties: general comments

- Uncertainties are not errors (and vice versa),
- They are related to risks, quality of work, money, perception, fear, safety...

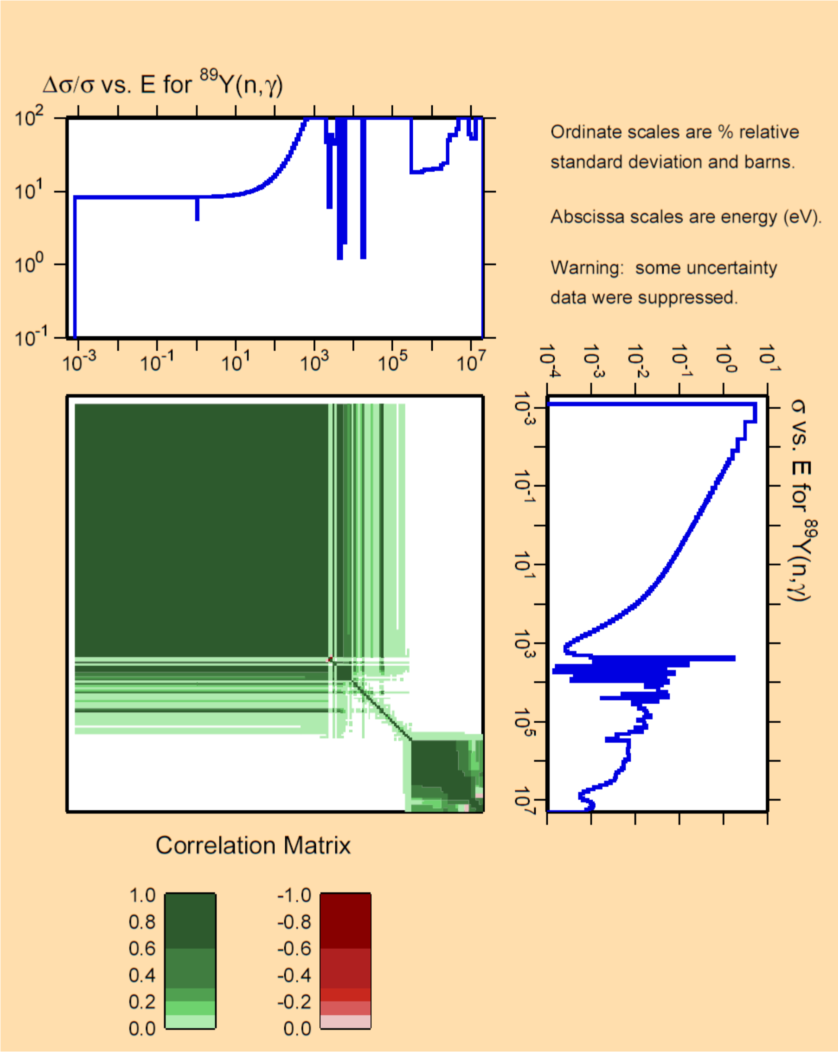
Uncertainty ⇌ safety ⇌ professionalism

- True uncertainties do not exist ! They are the reflection of our knowledge and methods.

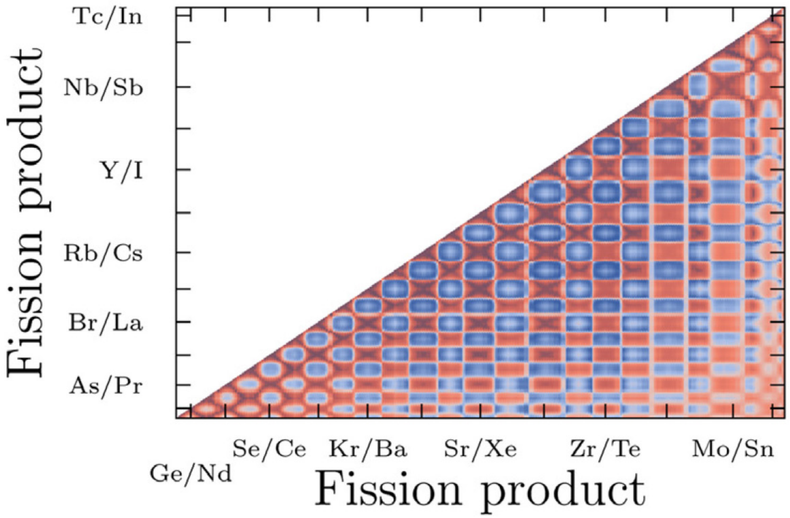
- All the above for covariances
- The importance of nuclear data uncertainties should be checked. If believed negligible, please prove it !

- Our motivation: Any justification for not providing uncertainties should become obsolete

Nuclear data uncertainties: examples



^{89}Y(n,g)



$^{235}\mathrm{U}+n_{\mathrm{th}}$

Uncertainty propagation

Three methods exist today:

1. Based on nuclear data covariance data
- So-called "Sandwich rule" = sensitivity times covariances ,
- Provide uncertainties, sensitivities

2. Based on nuclear data parameter covariance data:
- So-called TMC (Total Monte Carlo)
- Sampling of model parameters,
- Provide uncertainties,
- Does not provide sensitivities, but importance factors.

3. In between: based on nuclear data covariance data:
- Sampling of cross section data, based on nuclear data covariances
- Provide uncertainties,
- Does not provide sensitivities, but importance factors,
- Many software: XSUSA, ACAB, NUDUNA, NUSS, SANDY, SAMPLER…

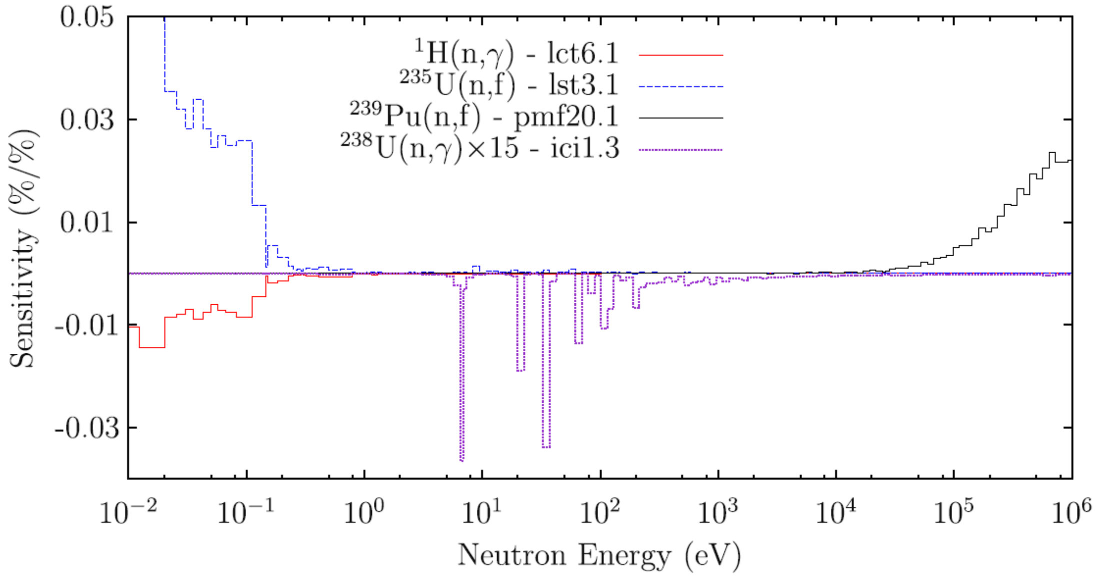
Uncertainty propagation: Sandwich rule

$$\sigma_R^2 = \sum_{i,j} S_i^R C(\alpha_i \alpha_j) S_j^R = \vec{S} C \vec{S}^T , \qquad (1)$$

Eq. (1) succinctly summarizes the information required to calculate the relative variance $\left(\sigma_R^2 = \left(\frac{\delta R}{R}\right)^2\right)$ of a linearized system response R as the product of the relative sensitivity coefficient $\vec{S}$ and the relative covariance matrix C of inputs (α_i), $i = 1, \ldots, N$, where

$$\vec{S} = (S_1^R, \ldots, S_N^R);\ S_i^R = \frac{\partial R}{R} \frac{\alpha_i}{\partial \alpha_i} ;$$

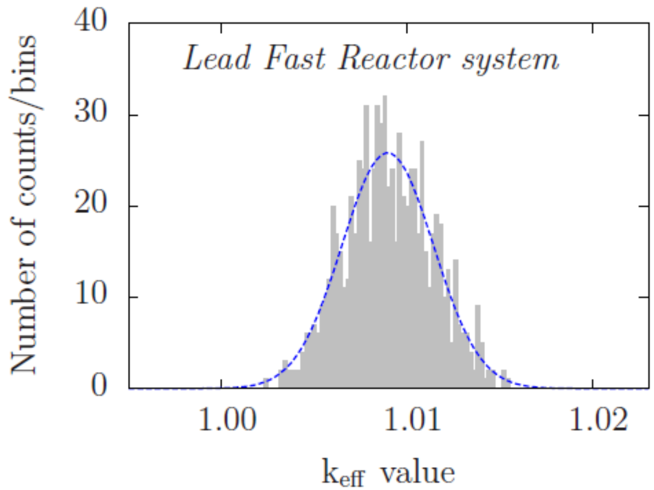
$$C(\alpha_i \alpha_j) = \frac{\mathrm{COV}(\alpha_i \alpha_j)}{\alpha_i \alpha_j} . \qquad (2)$$

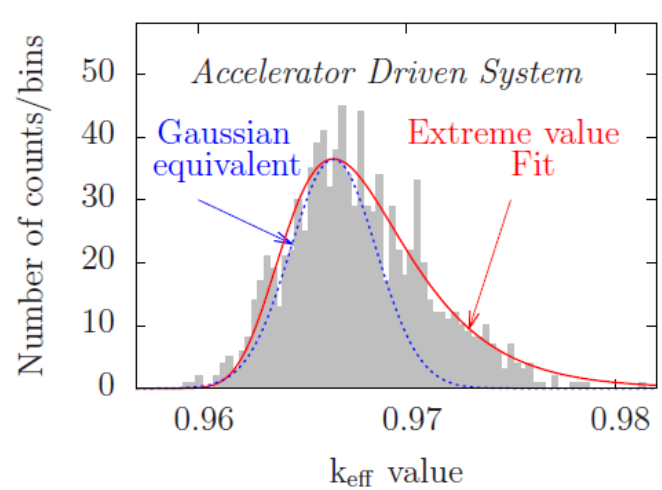


Uncertainty propagation: TMC

For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the n calculations, n different k_{eff} values are obtained.

$$\sigma^2_{\text{total}} = \sigma^2_{\text{statistics}} + \sigma^2_{\text{nuclear data}}$$





"Towards sustainable nuclear energy: Putting nuclear physics to work",
A.J. Koning and D. Rochman, ANE 35 (2008) 2024.

TMC for nuclear data uncertainty propagation, what else ?

☺ + No covariance matrices (no 2 Gb files) but every possible cross correlation included,

☺ + No approximation but true probability distribution,

☺ + Only essential info for an evaluation is stored,

☺ + No perturbation code necessary, only "essential" codes,

☺ + Feedback to model parameters,

☺ + Full reactor core calculation and transient,

☺ + Also applicable to fission yields, thermal scattering, pseudo-fission products, all isotopes (...just everything),

☺ + Other variants: AREVA (NUDUNA), GRS (XSUSA), CIEMAT (ACAB), PSI (NUSS), CNRS Grenoble..., based on covariance files,

☺ + Many spin-offs (TENDL covariances, sensitivity, adjustment...)

☺ + Computer time (not human time)

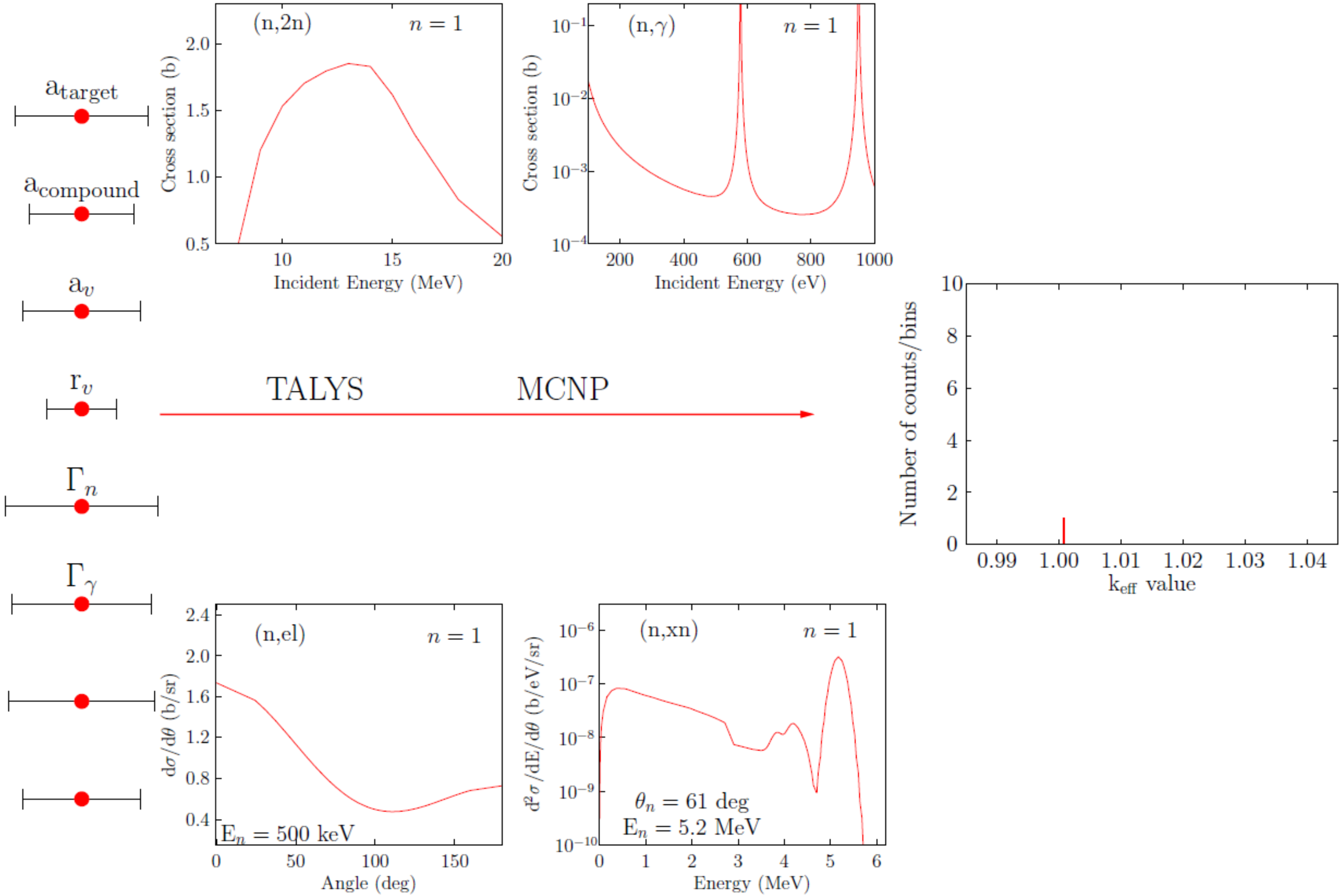
☺ + QA.

☹ - Needs discipline to reproduce,

☹ - Memory and computer time (not human time),

☹ - Need mentality change.

Hands on “1000 ×(TALYS + ENDF + NJOY + MCNP) calculations”



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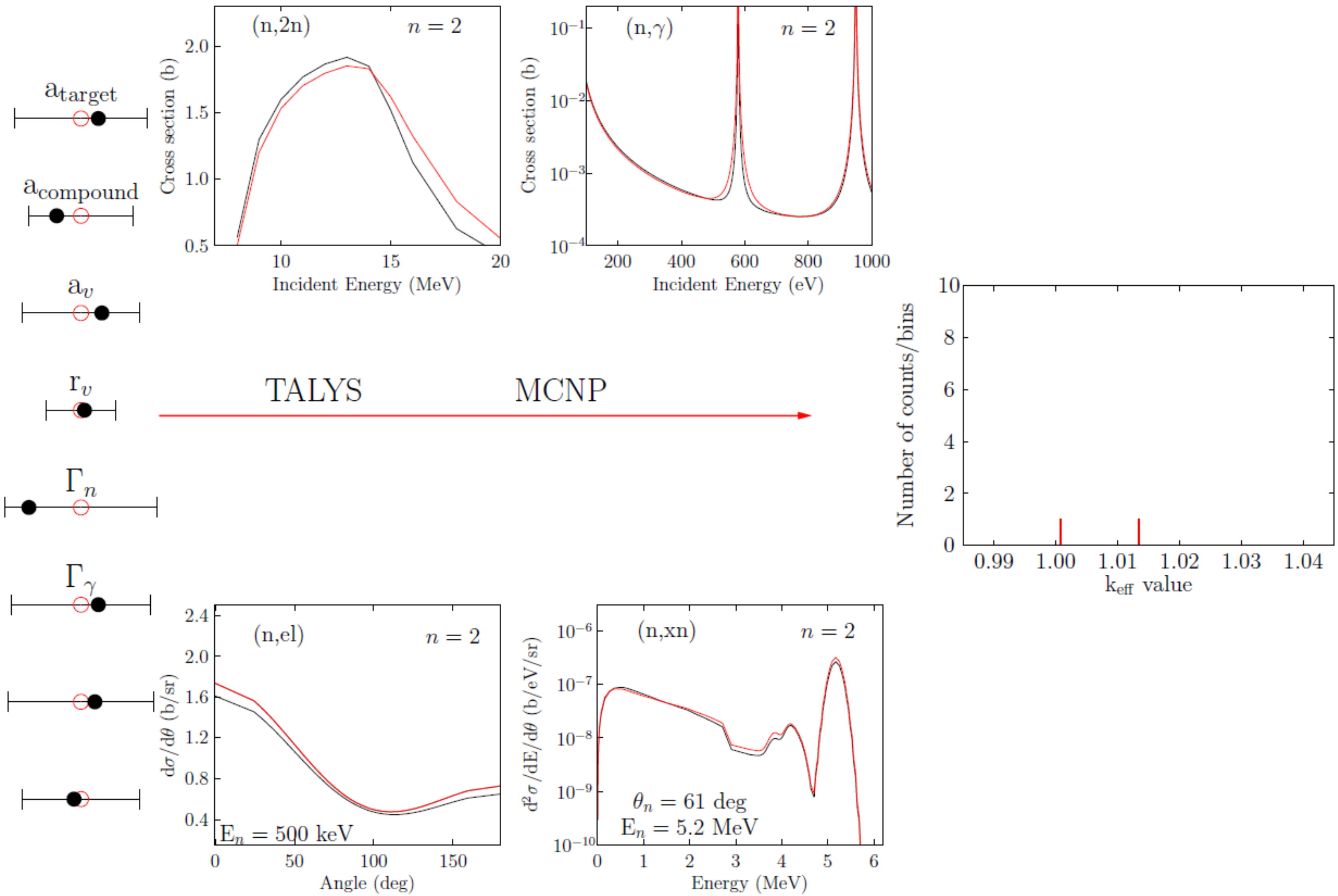

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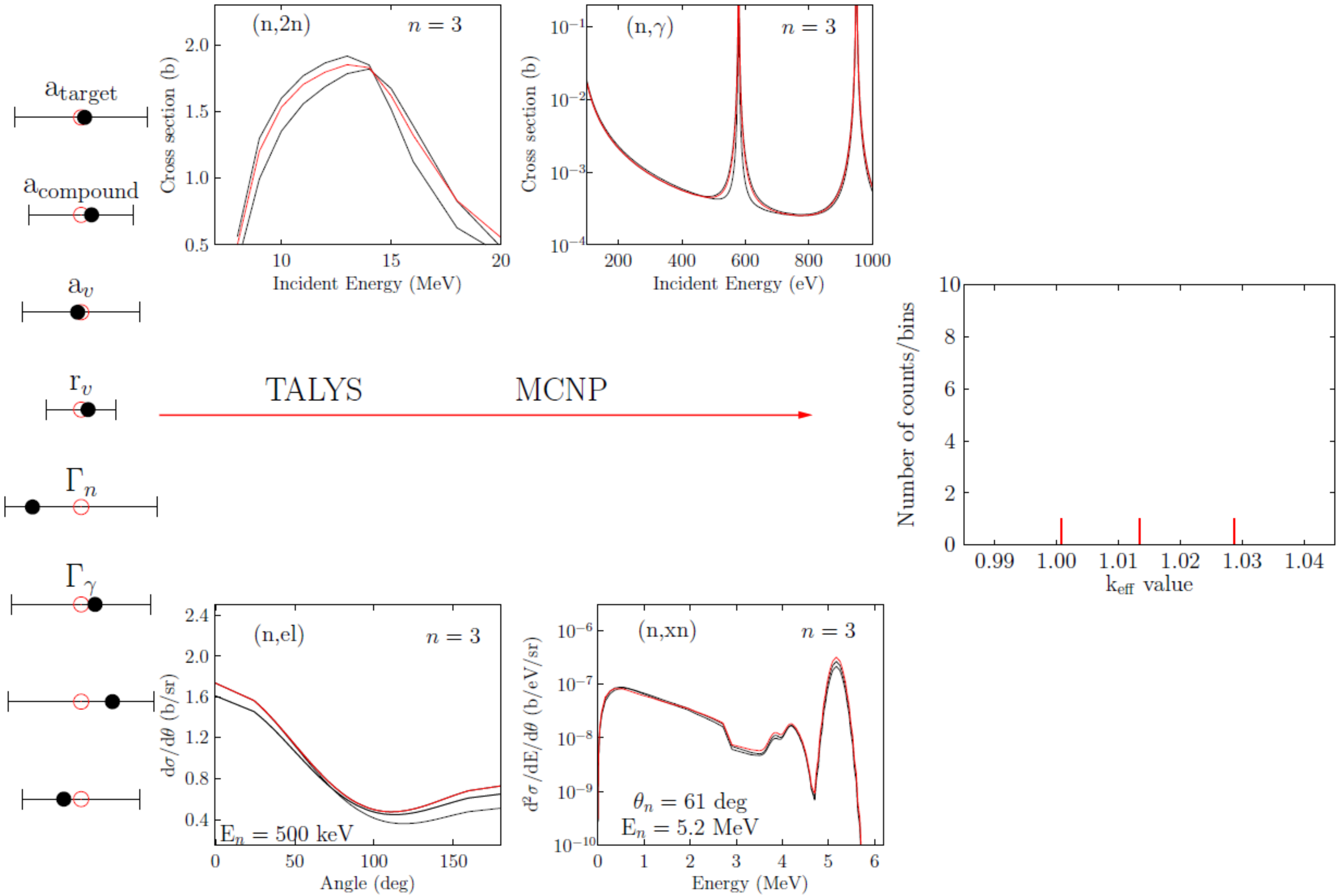

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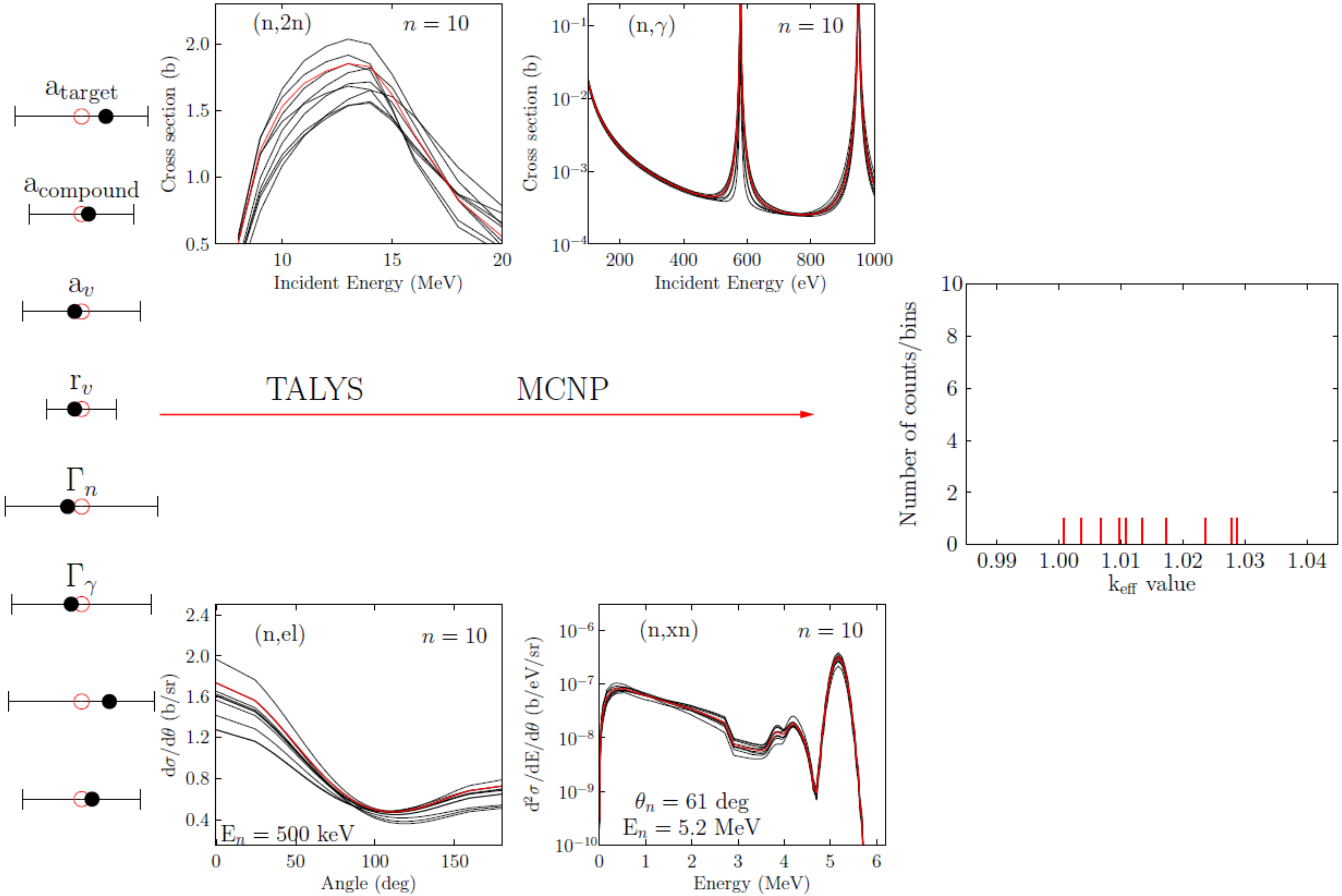

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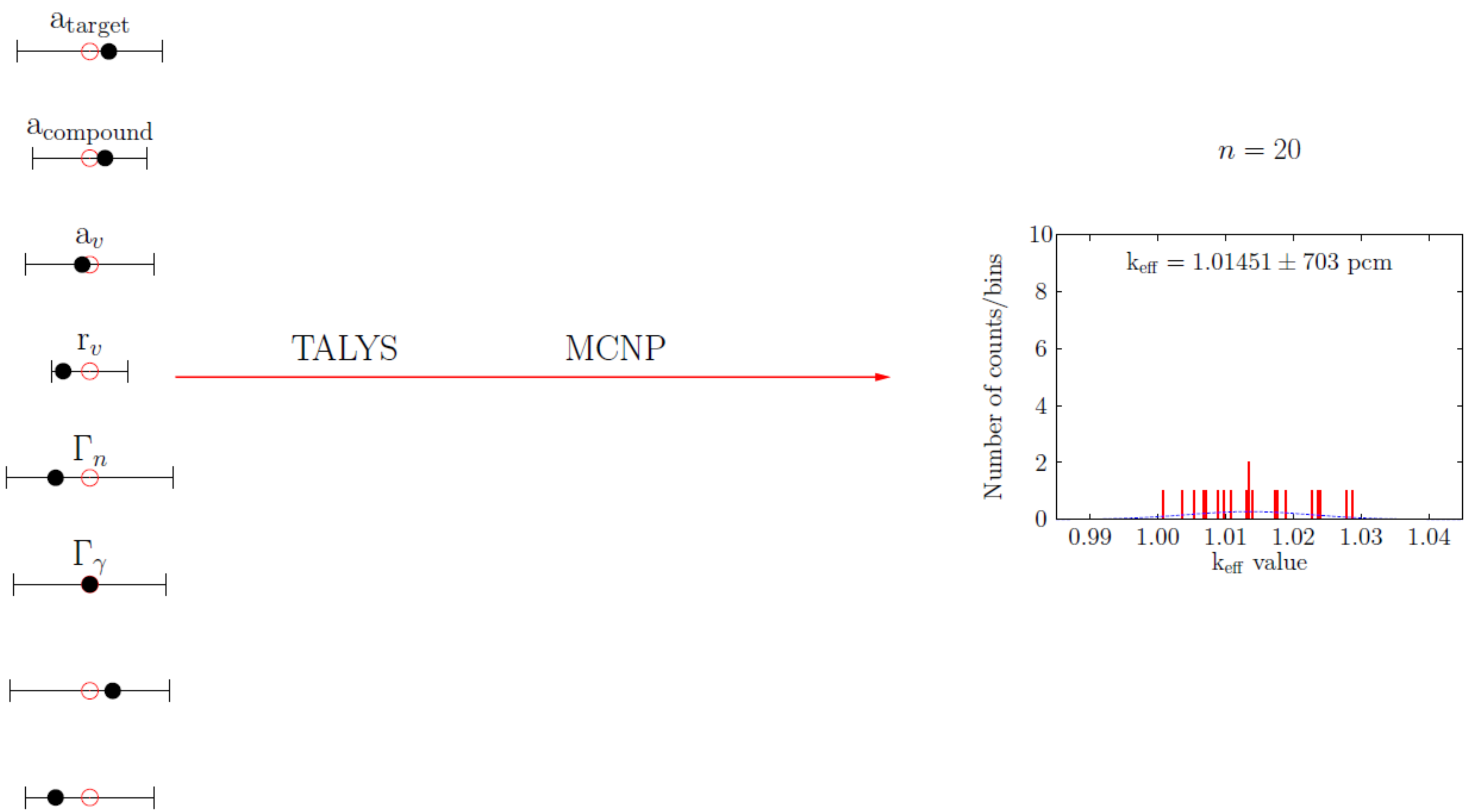

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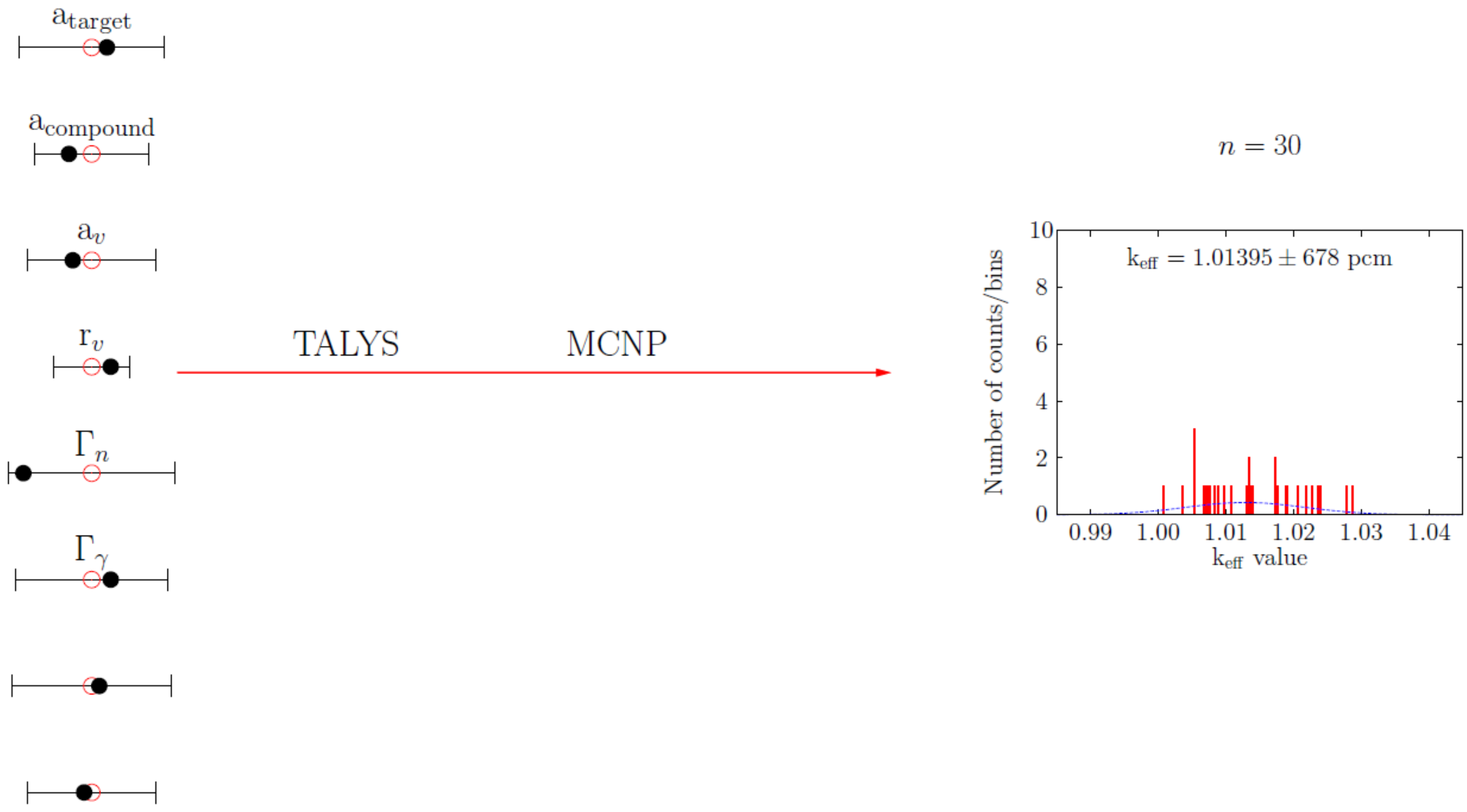

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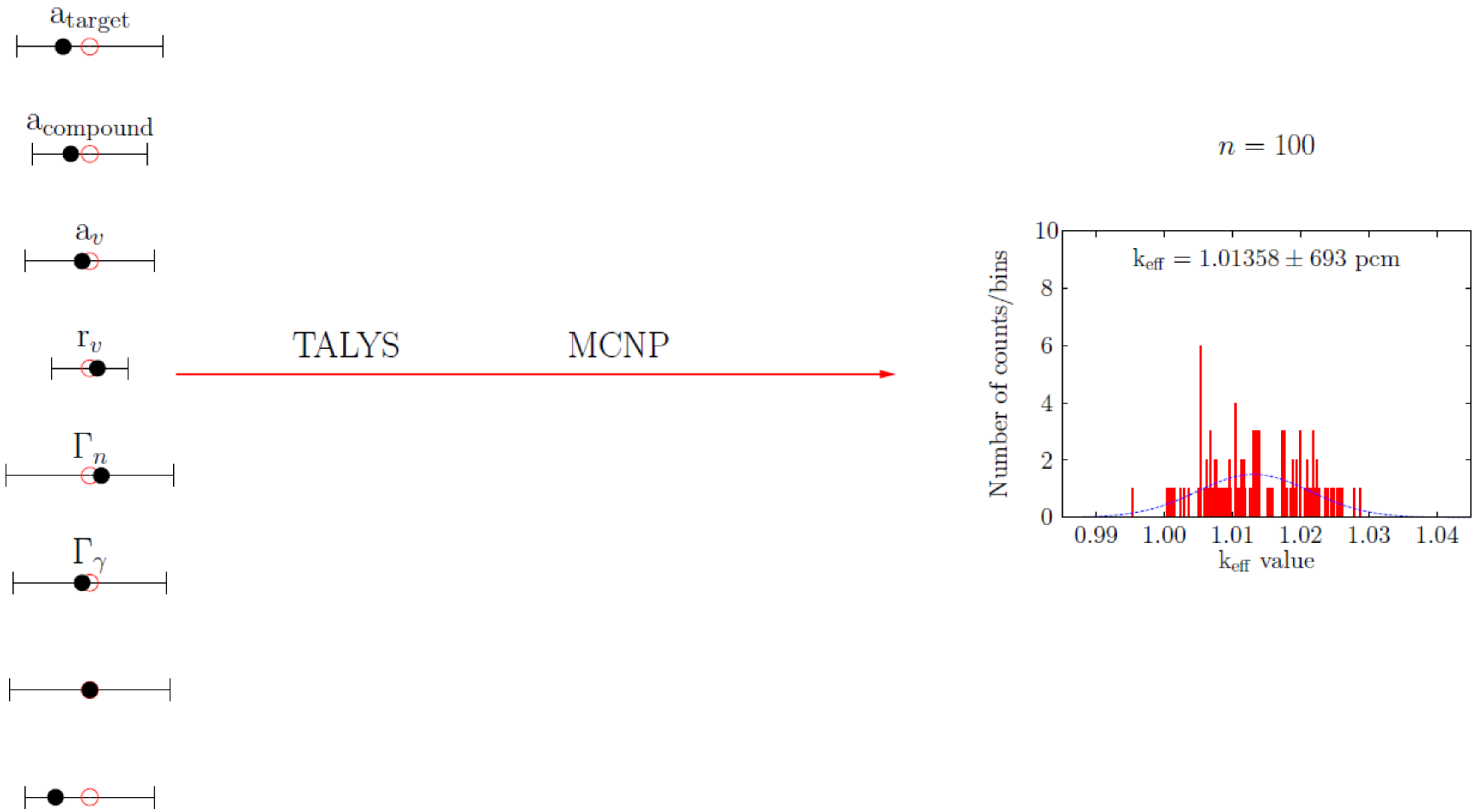

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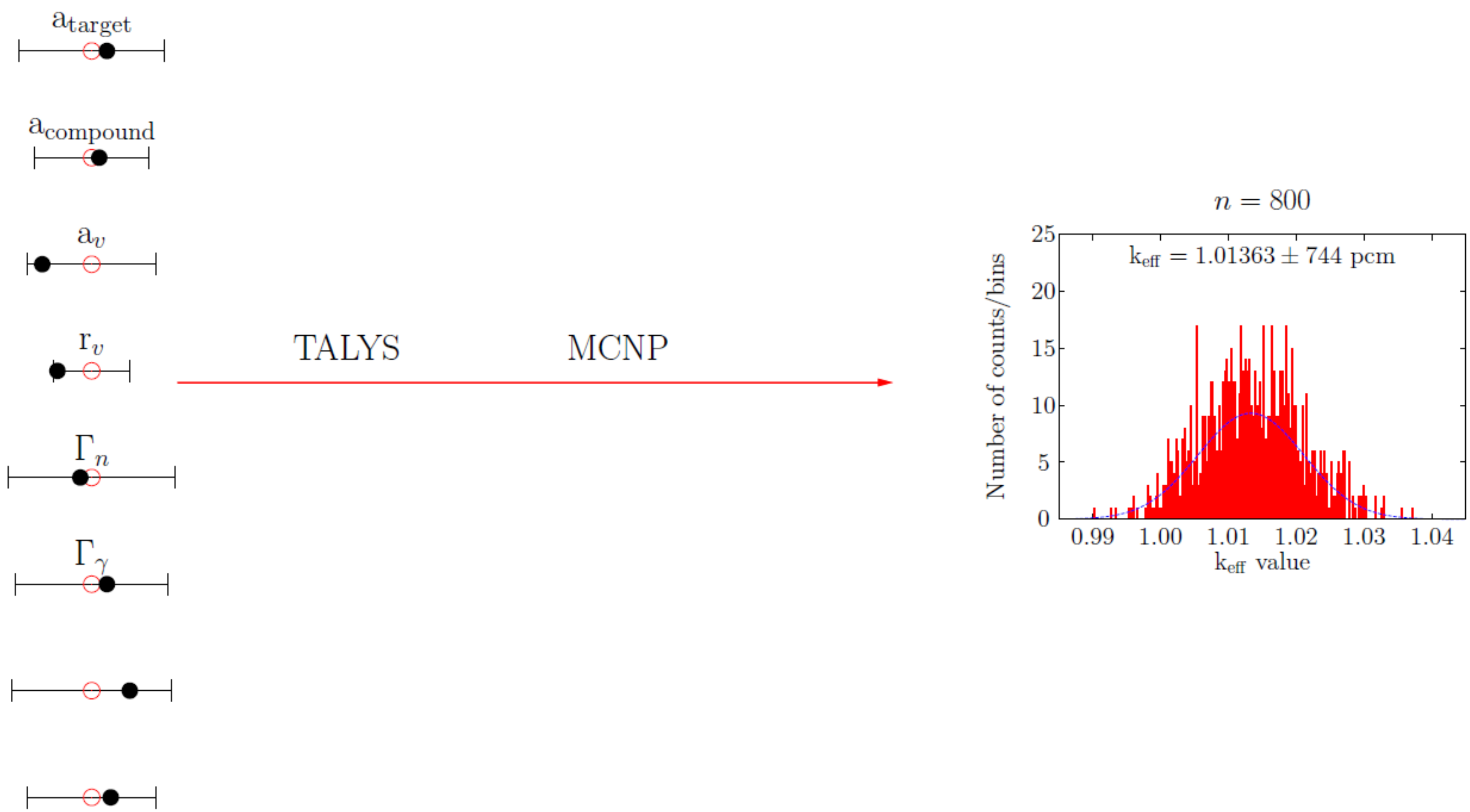

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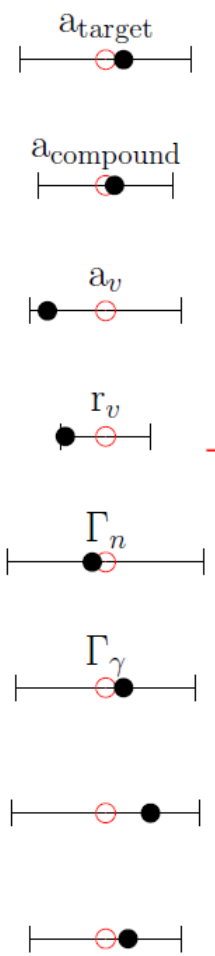
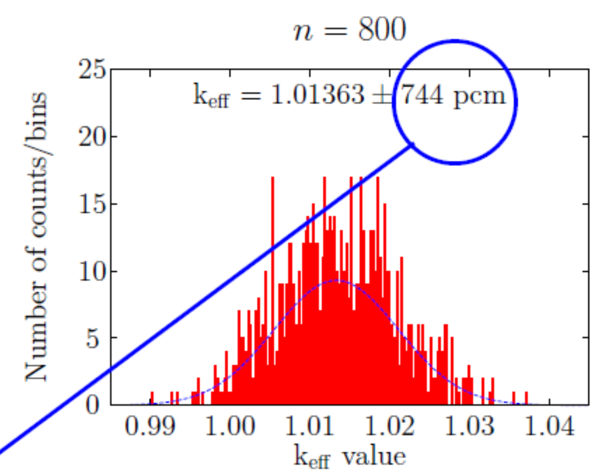


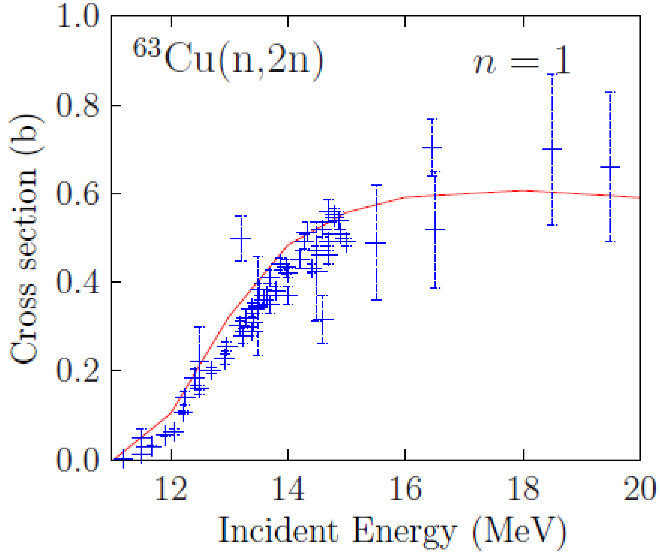
TALYS MCNP

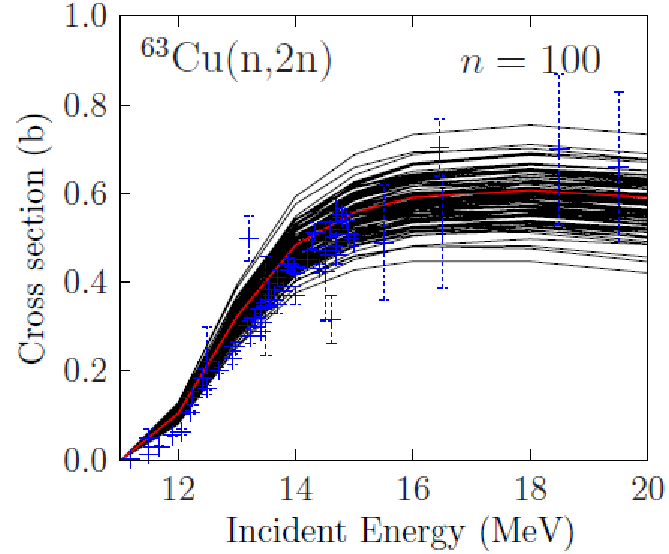


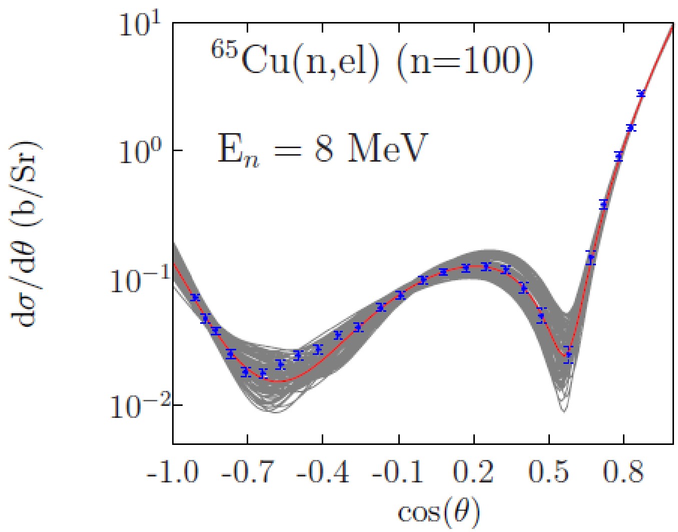
Statistical uncertainty $\simeq$ 68 pcm

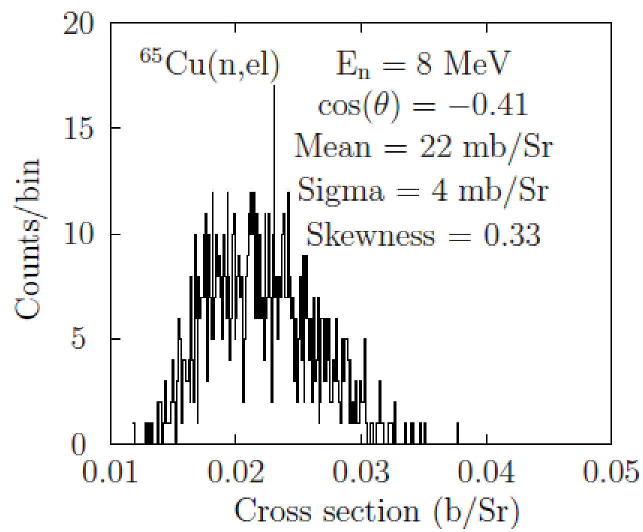
$\Longrightarrow$ uncertainty due to nuclear data $\simeq$ 740 pcm

Examples with ^{63}Cu(n,2n) and ^{65}Cu(n,el)

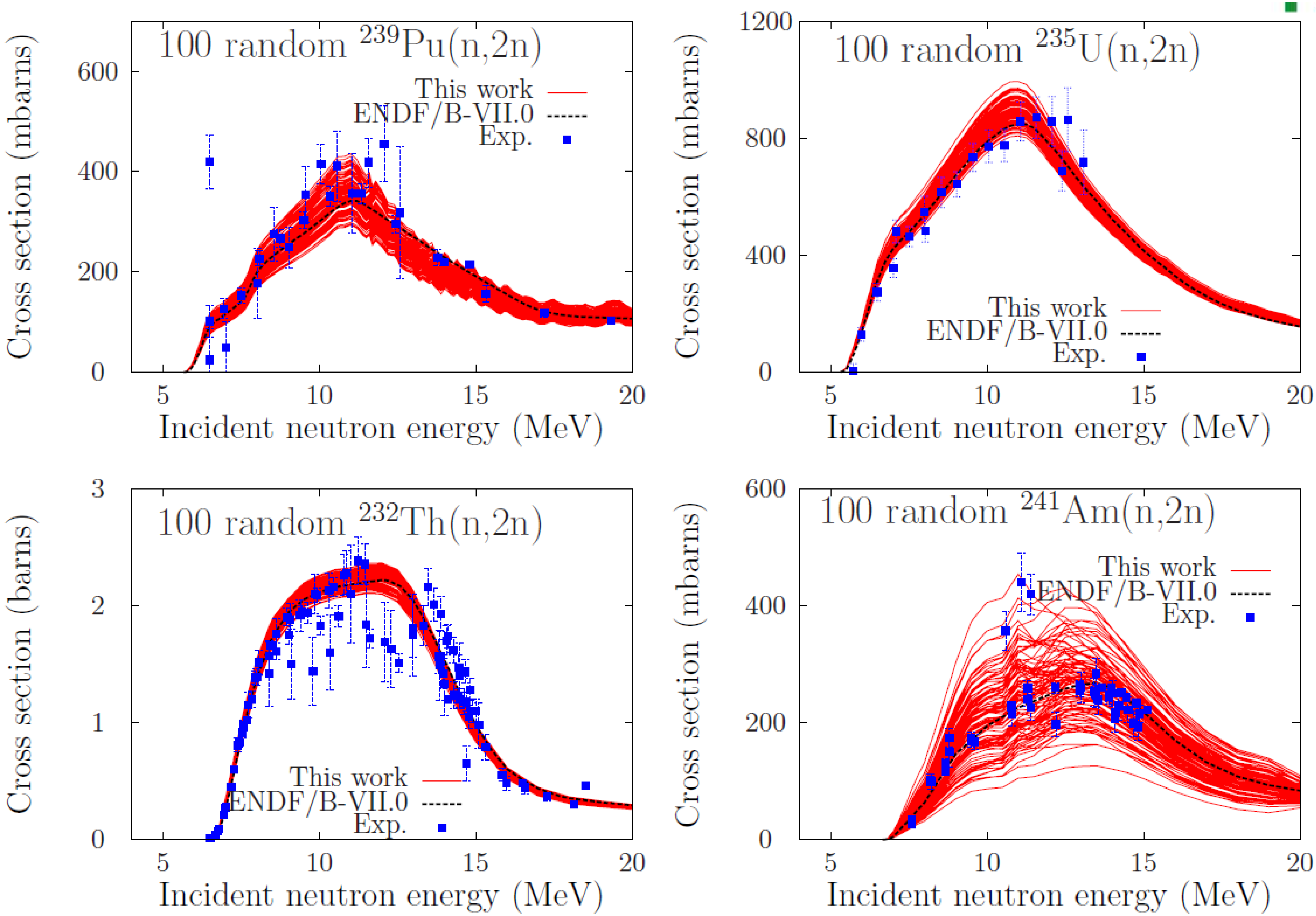




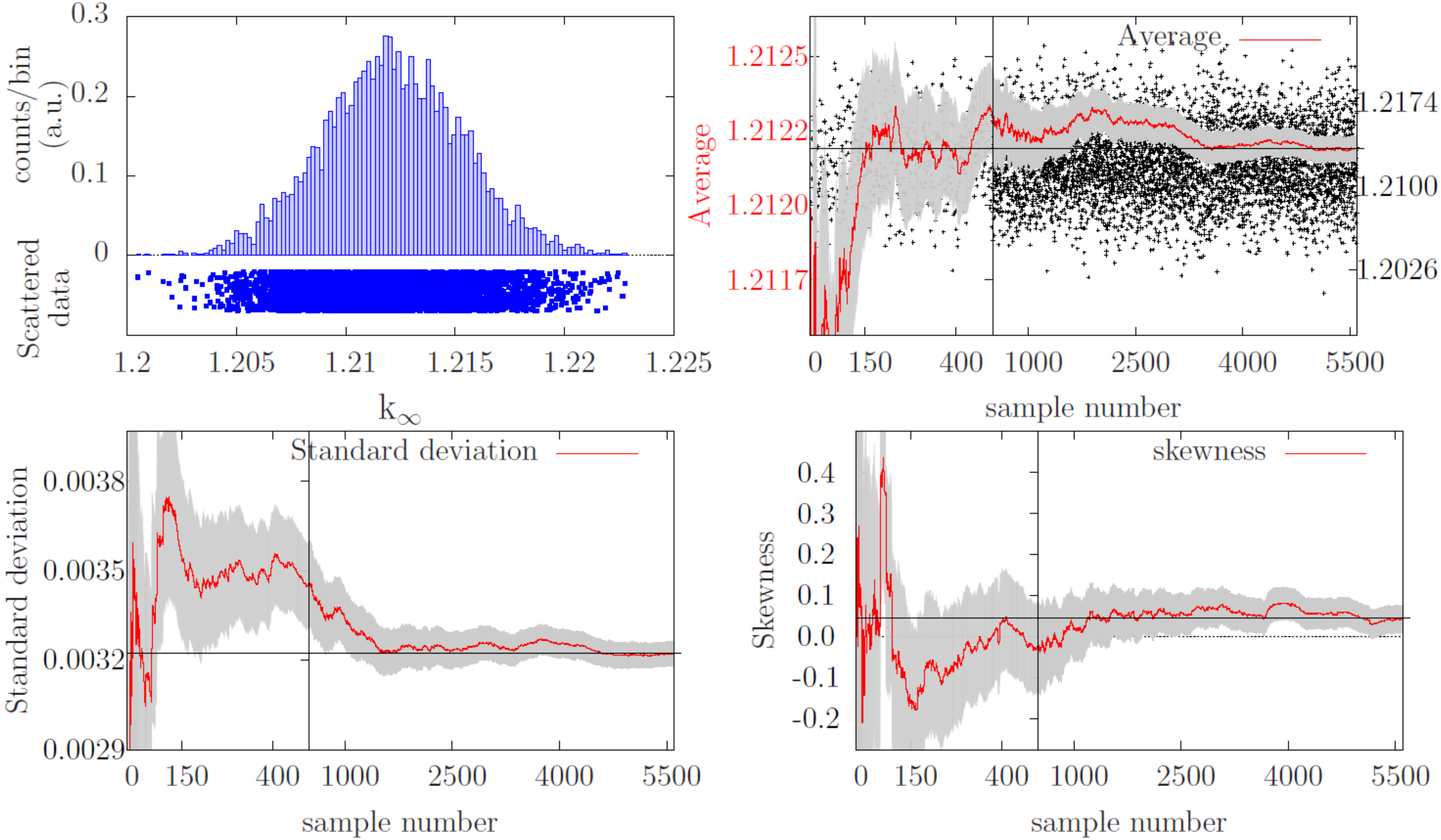




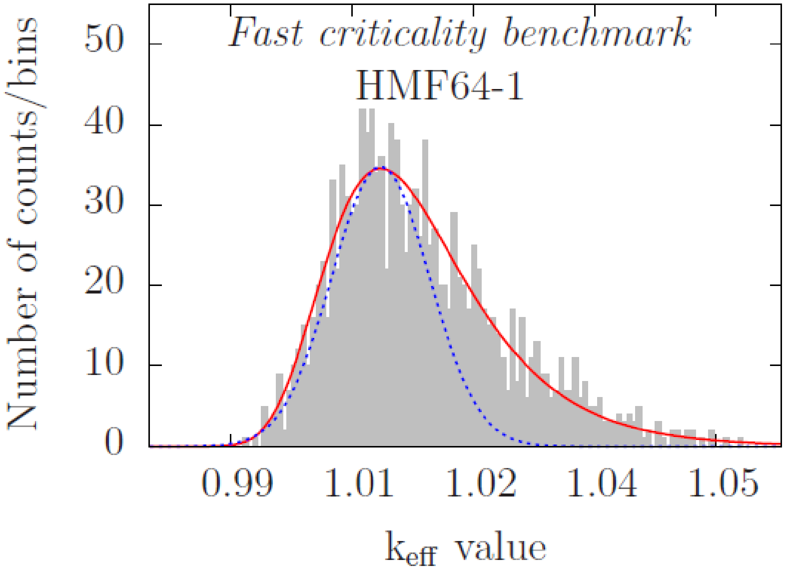
Nuclear data: examples on (n,2n) cross sections

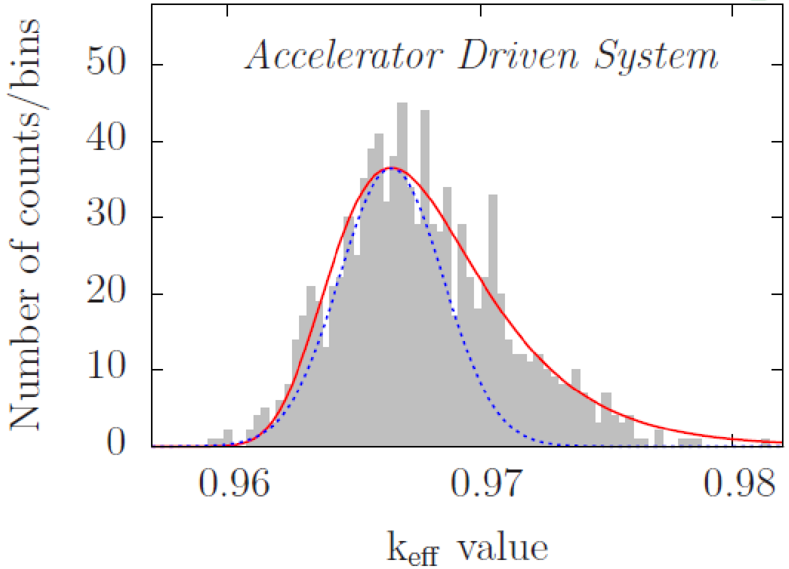


TMC: Convergence of the Monte Carlo process



TMC: No Gaussian assumption





Better fit with the "*Extreme Value Theory*", or EVT:

$F(z) = e^{-z-e^{-z}}$ with $z = \frac{X-\mu}{\sigma}$

Mean $\mu' = \mu + \gamma\sigma$

Standard Deviation $\sigma' = \sigma\frac{\pi}{\sqrt{6}}$

	HMF-64.1	ADS
k_{eff}	1.00848 μ'=1.01394	0.96648 μ'=0.96785
$\sigma_k \times 10^5$	**855** σ'=**1097**	**291** σ'=**345**

Conclusion on TMC

- Anyone can do it with the random nuclear data files from the TENDL website
- All types of nuclear data impact can be assessed,
- Most direct way to propagate uncertainties
- Better QA, better modern use of computers
- TMC is part of global approach to improve transparency and safety of nuclear simulation
- Fast TMC: Same as TMC, but all in the equivalent of a single running time,

TMC: If we can do a calculation once, we can also do it a 1000 times, each time with a varying data library

Fast TMC: If we can do a calculation once, we can also get nuclear data uncertainties at the same time

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Wir schaffen Wissen – heute für morgen