Nuclear data uncertainty propagation using a Total Monte Carlo approach

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Europe by night
NRG
Petten

Petten site

http://www.nrg.eu

Complete infrastructure in Petten

Actinide lab

(~10 in the world)

Large Test Reactor

(~10 in the world)

Hot Cells

(~20 in the world)

Combination = Unique in the world

fabrication recycling material

irradiation in HFR

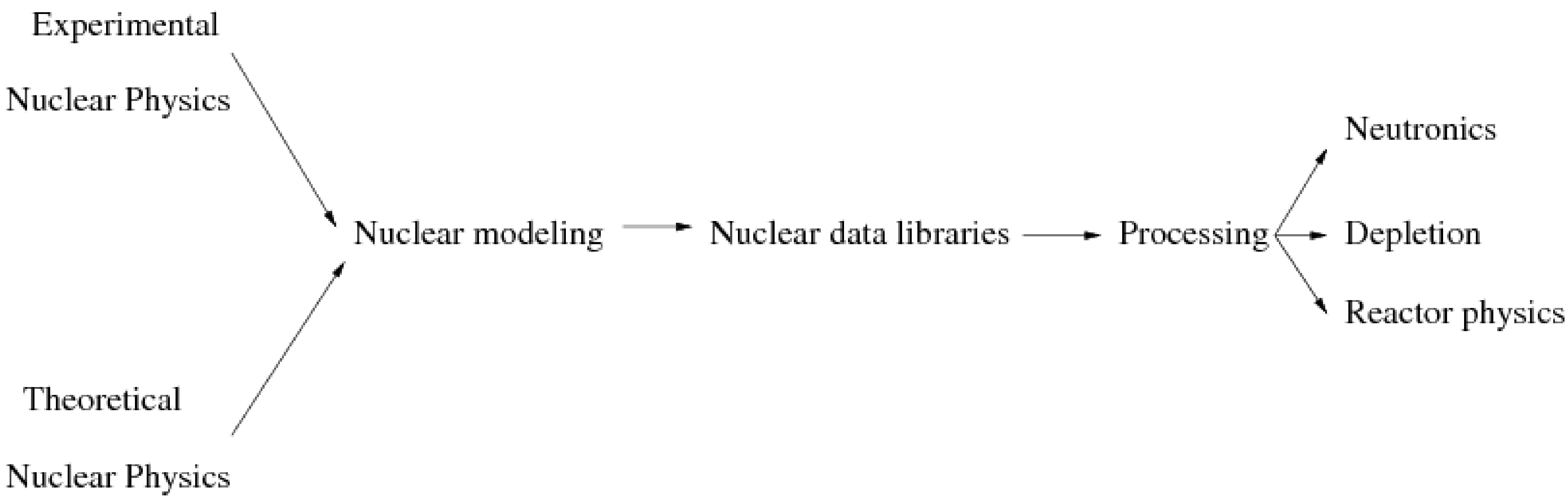
post irradiation examination in hot cell laboratories

And we combine this with nuclear computational simulations!

Contents

- Introduction
- Full control over nuclear data + uncertainty propagation + reactor calculations – 4 stages:
    1. Create the best possible nuclear data library: TENDL
    2. Validate TENDL against integral experiments and benchmarks
    3. Perform Total Monte Carlo around the central values of TENDL for uncertainty propagation in reactor analyses
    4. Generalize Total Monte Carlo methodology to full core analyses
- Conclusions

Automating nuclear science



Road to success:

- Use (extremely) robust software
- Store all human intelligence in input files and scripts
- Rely on reproducibility and quality assurance

Strategy

1. Create the best possible nuclear data library (TENDL) using:
   - Experimental data (EXFOR database)
   - The TALYS nuclear model code
   - Resonance information (TARES code)
   - Pick and choose from existing nuclear data libraries (ENDF/B-VII, JEFF, etc.)
2. Validate TENDL against open-source integral experiments and benchmarks:
   - ICSBEP criticality benchmarks
   - SINBAD shielding benchmarks
   - IRPHE reactor benchmarks
   - Activation and decay heat experiments

This establishes the central values, i.e. a “normal” nuclear data library.

Strategy

3. Randomize nuclear data around the central values of TENDL to perform Total Monte Carlo:
   - Obtain exact uncertainties for criticality benchmarks etc.
   - Perform reactor/burnup calculations on pin cell and assembly level including uncertainties
   - The ‘Petten Method’: Monte Carlo optimization of nuclear data
4. Generalize TMC methodology to full core calculations
   - Generate random nuclear data libraries for PANTHER, CASMO-SIMULATE, RELAP etc.
   - Perform dynamical calculations, transient and thermohydraulics, including uncertainties

If 1-4 are successful, we have the best central nuclear data values *and* the most flexible and exact uncertainty methodology

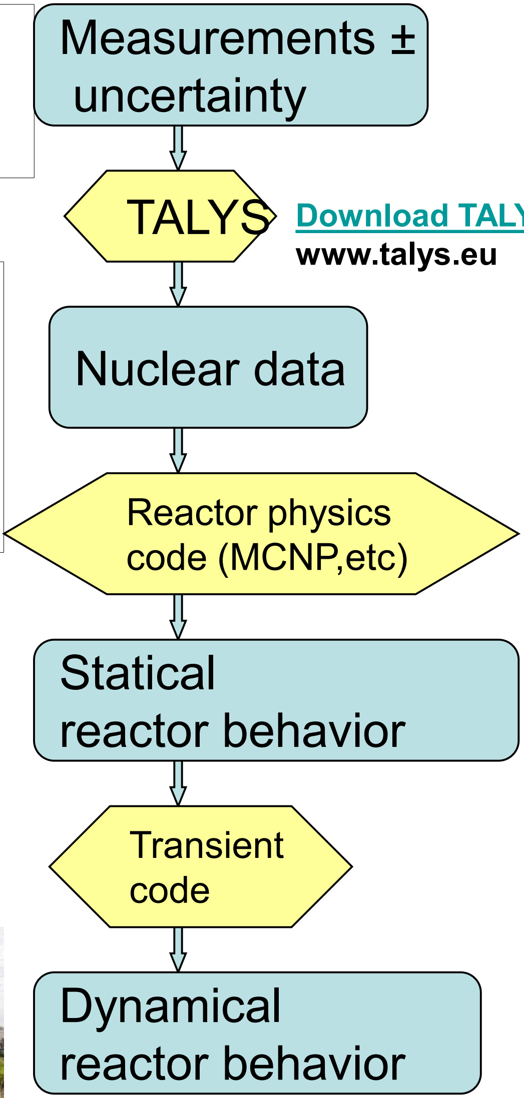
Safety and sustainability – nuclear data

Starting point: basic nuclear data for reactor and fuel cycle analyses have uncertainties

Required: insight in how uncertainty of nuclear data is propagated to nuclear energy safety and sustainability issues.

Observation: the world is working hard to yield answers to this within 10-20 years.

Claim : it can be done faster than that using TALYS



Download TALYS-1.4!
www.talys.eu

TALYS Evaluated Nuclear Data Library: TENDL-2012

- Neutron, proton, deuteron, triton, helium-3, alpha and gamma data libraries.
- 2430 targets (all isotopes with lifetime > 1 sec.)
- Complete reaction description in ENDF-6 format: MF1-MF40, up to 200 MeV
- MCNP-libraries (“ACE-files”), PENDF files and multi-group covariance data

Default: Global calculations by TALYS-1.48 and TARES (resonances)

which are overruled by

Adjusted TALYS calculations (340 input files) and Resonance Atlas-based TARES calculations

which are overruled by

TALYS-normalization to ~200 (experimental) evaluated reaction channels from other libraries (e.g. IRDFF, light nuclides, main channels of ^{235,238}U, ^{239}Pu)

TALYS

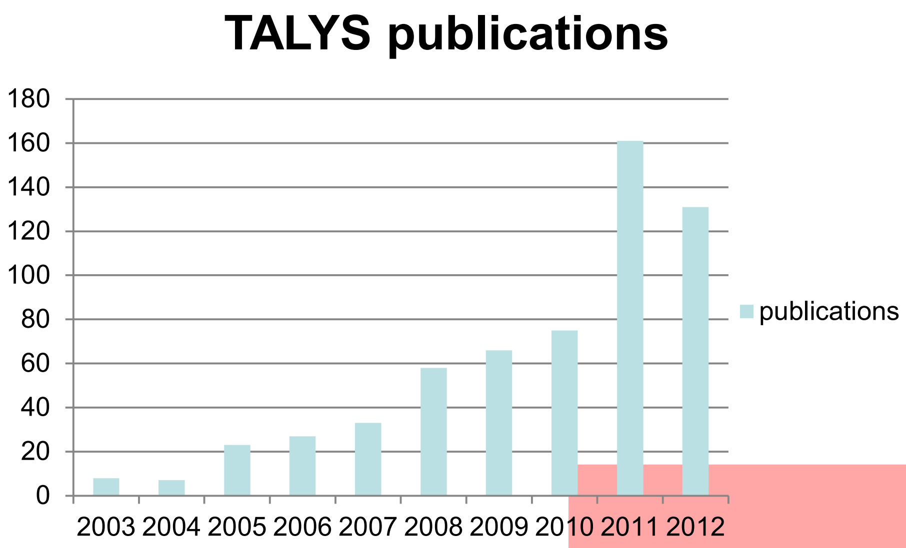
- Nuclear model code by NRG Petten, CEA-BRC, UL Bruxelles
- (Almost) Complete nuclear reaction input and output.

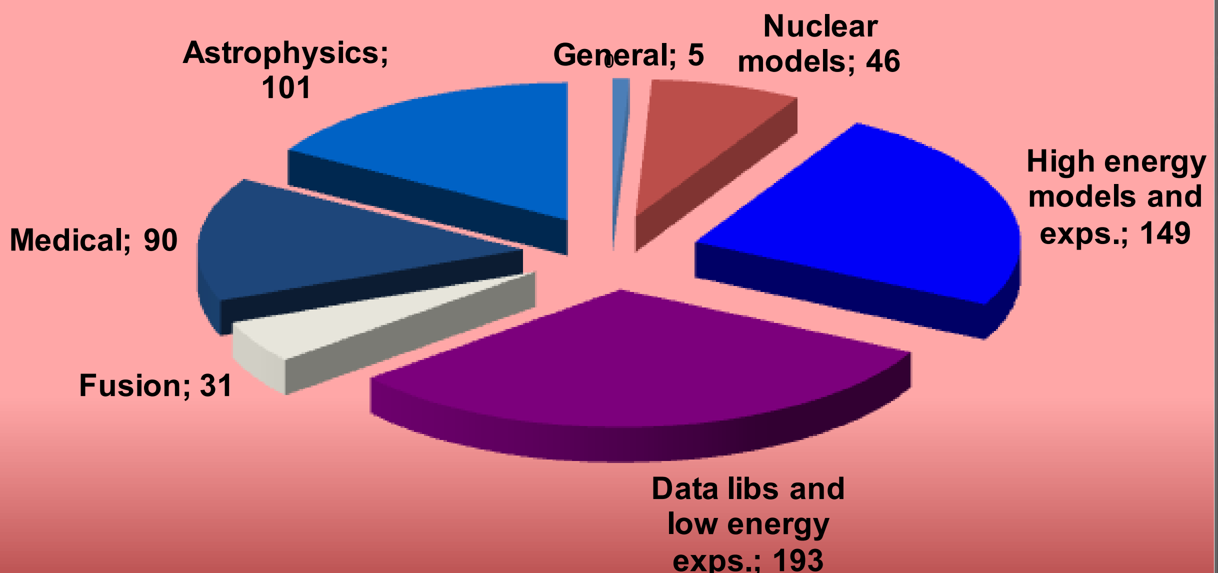
Release:

- www.talys.eu
- Latest official version, TALYS-1.4, released december 23, 2011.

Software issues:

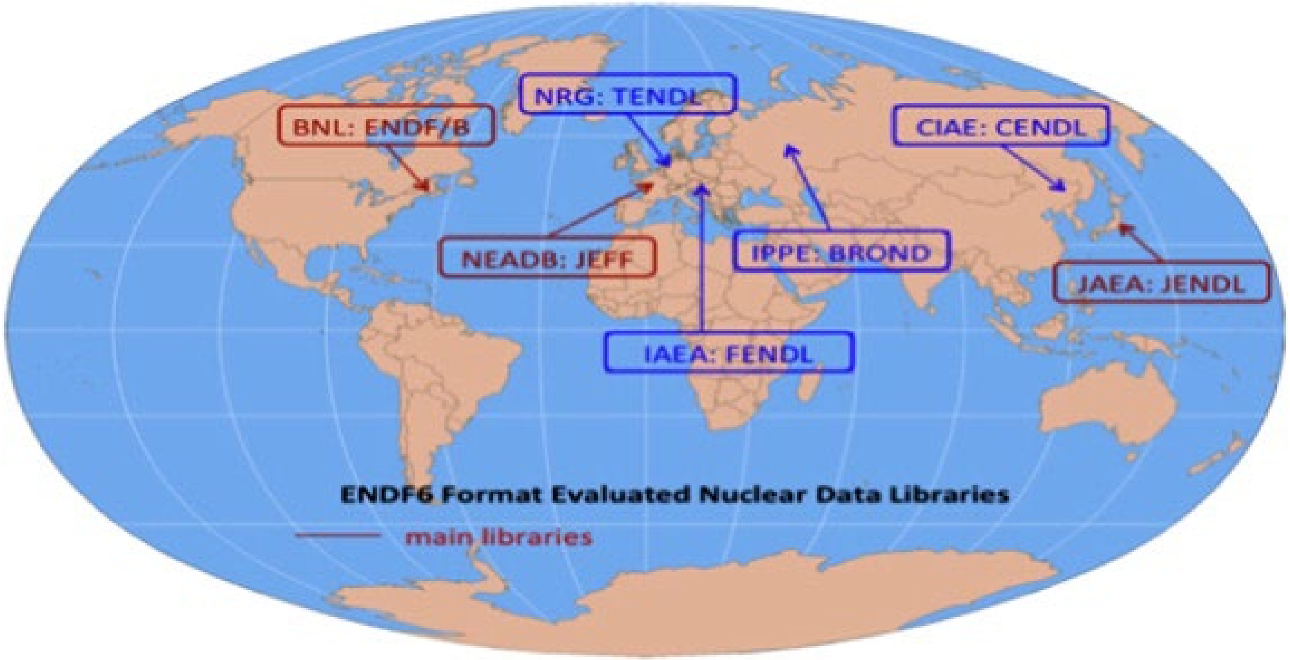
- Most used nuclear reaction code in the world
- Very flexible in use, robust, and readable consistent programming
- 300 page manual, 20 widely varying sample cases
- TALYS: open source
  - 600-800 users worldwide, who give valuable feedback
- Nuclear data software around TALYS (i.e. the step to technology): NRG proprietary


TALYS publications
180
160
140
120
100
80
60
40
20
0
2003 2004 2005 2006 2007 2008 2009 2010 2011 2012
publications


Astrophysics; 101
General; 5
Nuclear models; 46
High energy models and exps.; 149
Medical; 90
Fusion; 31
Data libs and low energy exps.; 193

Nuclear data libraries for nuclear technology

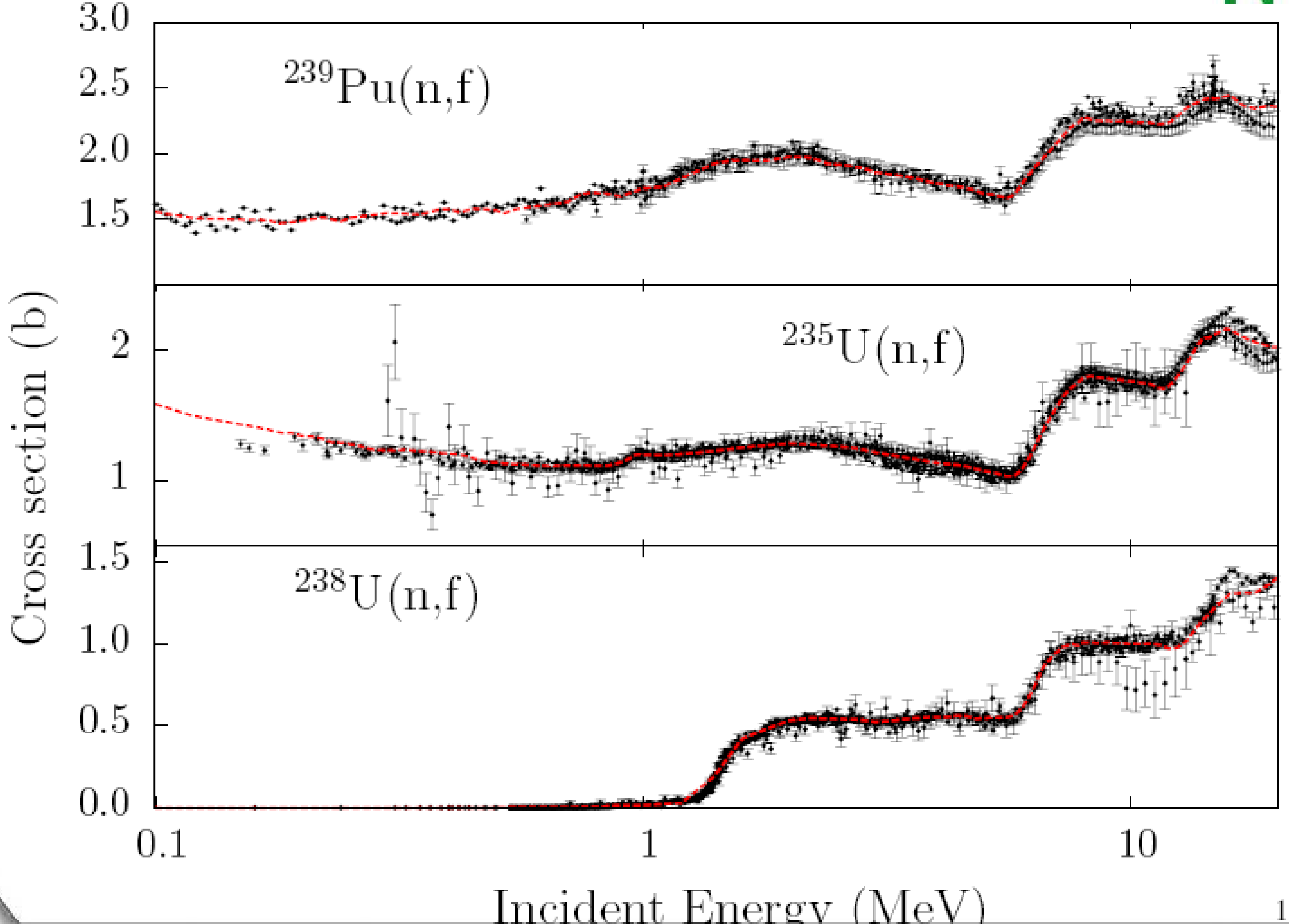
E. Sartori, Nuclear data for radioactive waste management, Ann. Nuc. En (2013).



Ken Kozier, AECL, IAEA meeting on long-term data needs, 2011

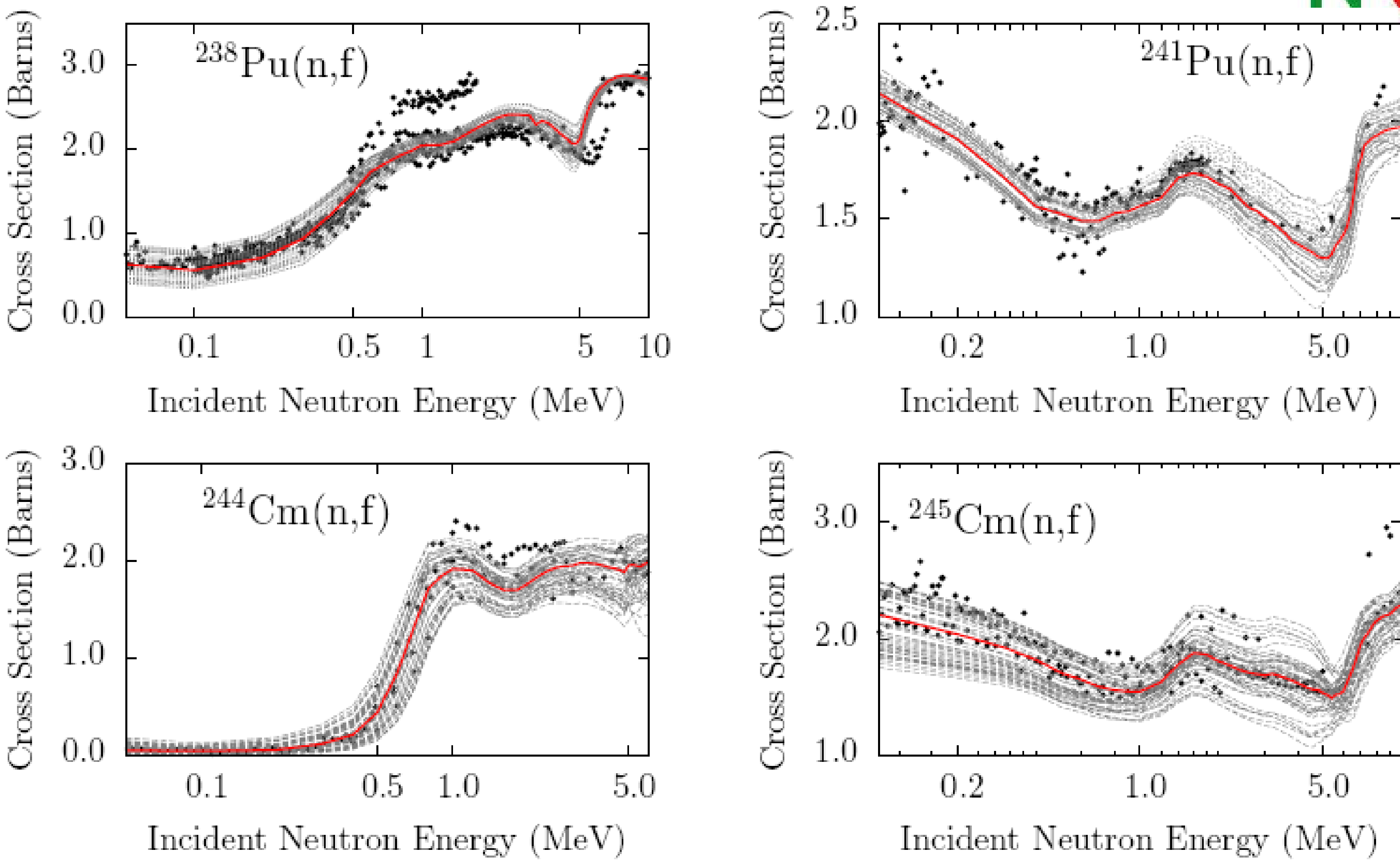
"The TALYS/TENDL system has rapidly evolved to be a likely candidate to form the basis for a single, global evaluated nuclear data library system. …. In the event that TALYS/TENDL continues to emerge as an unchallenged global contender, it is recommended that the IAEA provide moral and other support …"

Examples 3: Some actinides

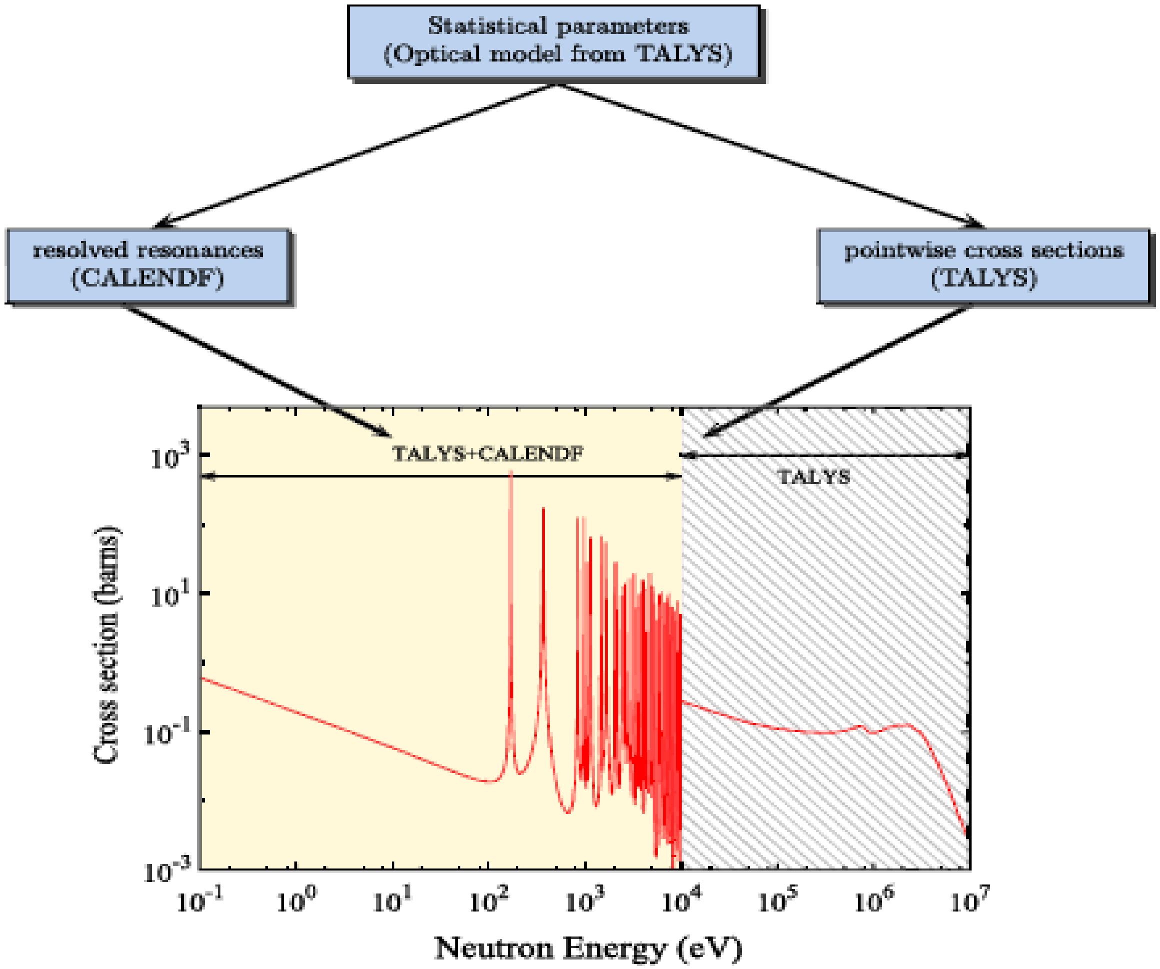


Covariances: example

23:22:46



High Fidelity Resonances (HFR)



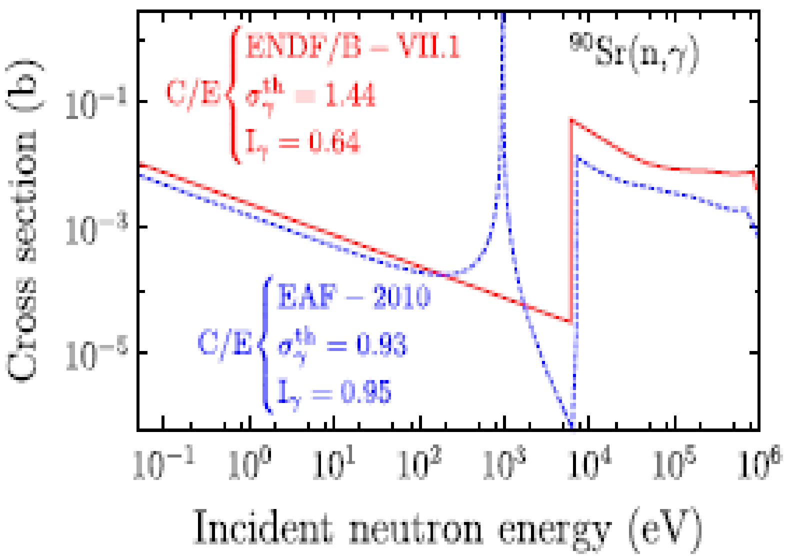
URR derived resonance ladders:

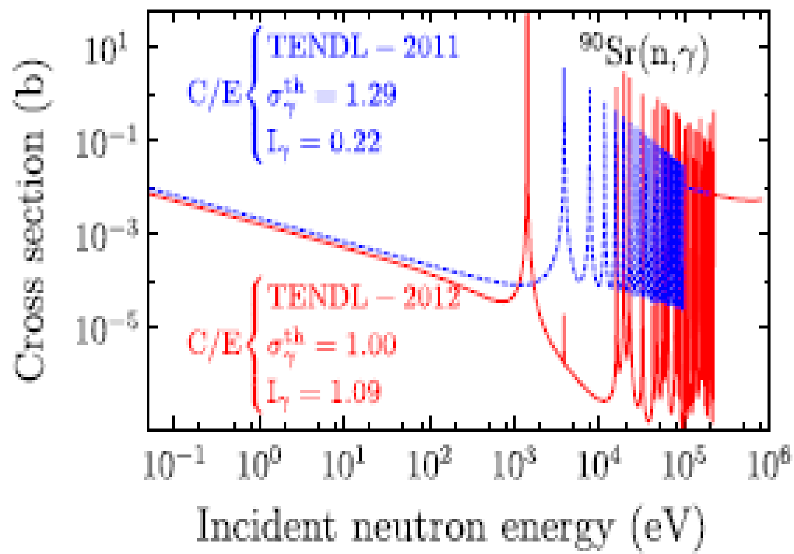
GOE for each (j,l)

Wigner law for spacing

KD03 OMP for average parameters

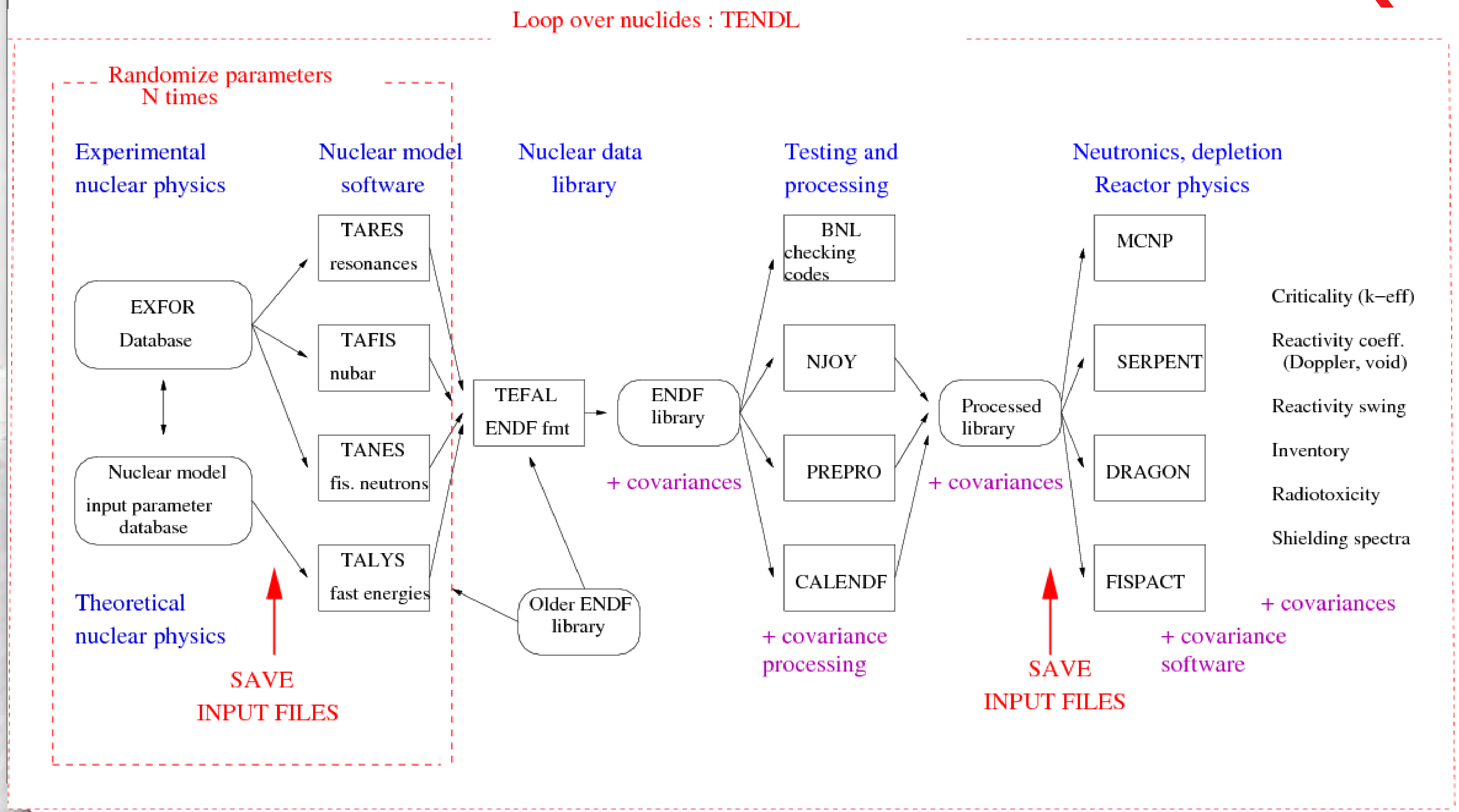
HFR





D. Rochman, A.J. Koning, J. Kopecky, J.-C. Sublet, P. Ribon and M. Moxon, ``From average parameters to statistical resolved resonances'', Ann. Nuc. En. 51, 60 (2013).

TENDL nuclear data library

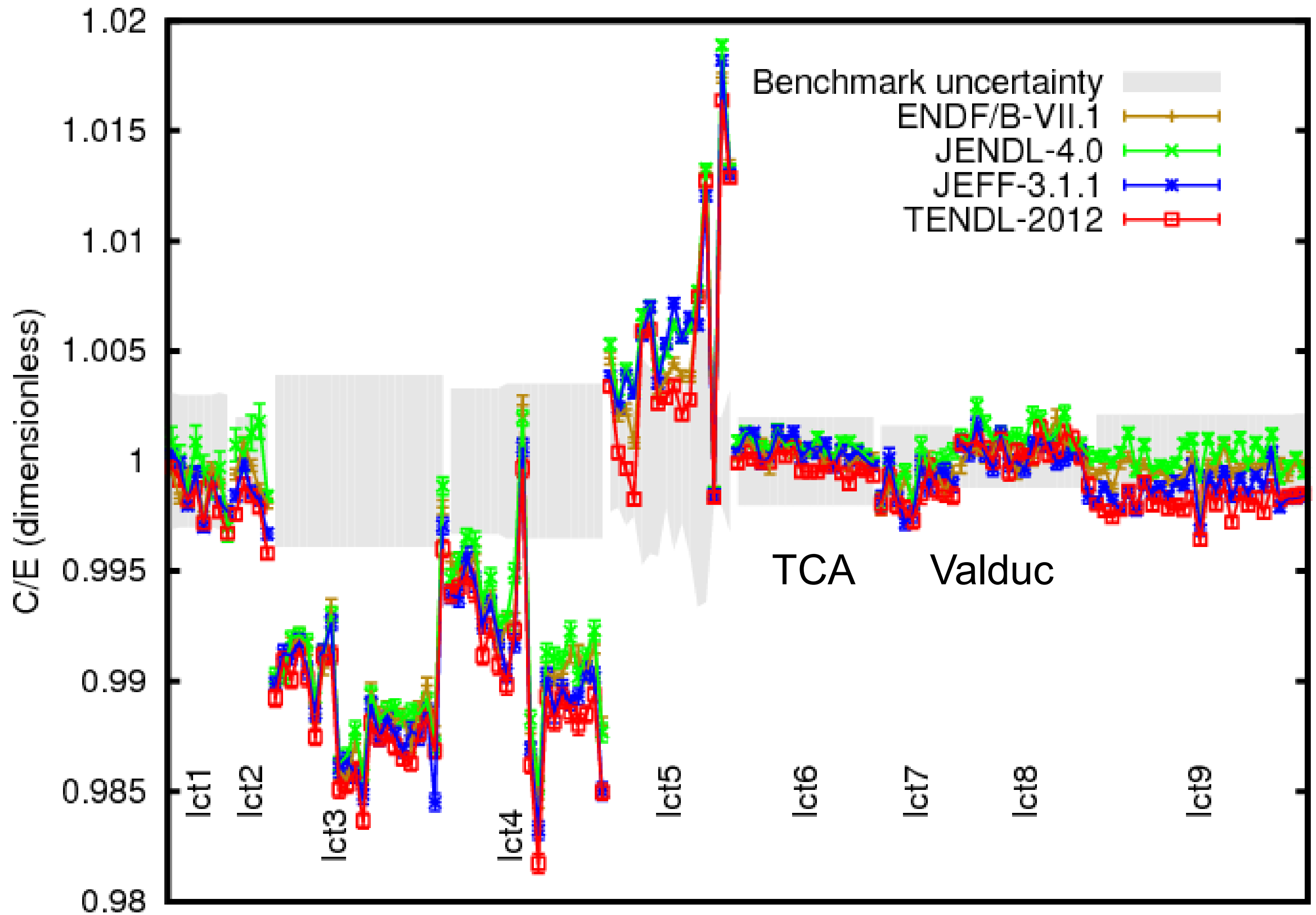


A.J. Koning and D. Rochman ,"Modern nuclear data evaluation with the TALYS code system“, Nuclear Data Sheets, 113, 2841 (2012)

Testing TENDL - Criticality safety: ICSBEP

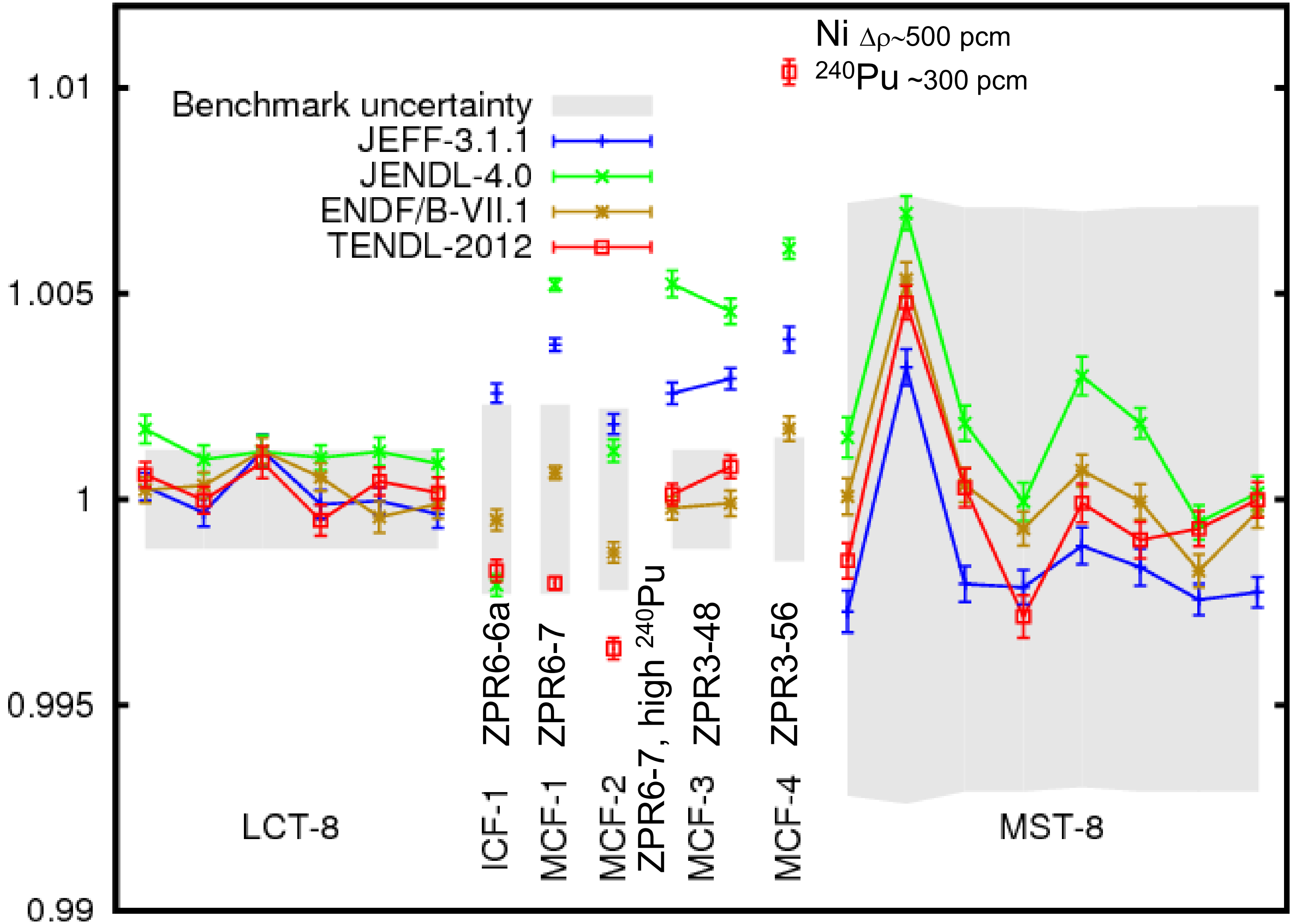
- International Criticality Safety Benchmark Evaluation Project
  - ✓ 516 evaluations, 4405 cases (2010 DVD)
- Type of fissile material
  - ✓ LEU, IEU, HEU, MIX, PU, ^{233}U
- Physical form of fissile material
  - ✓ Compound, Metal, Solution, Miscellaneous
- Neutron spectrum
  - ✓ Thermal, intermediate, fast, mixed

Criticality safety: leu-comp-therm



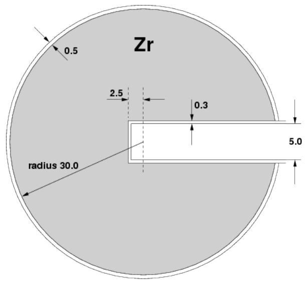
(S. van der Marck, ND-2013)

Criticality safety: Na

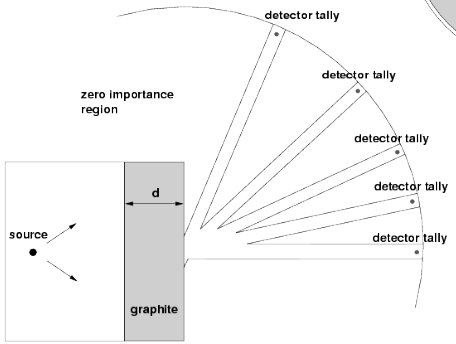


Shielding benchmarks

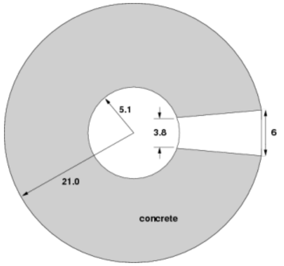
- Oktavian
  - ✓ LiF, Al, Si, Ti, Cr, Mn, Co, Cu, Zr, Mo, W



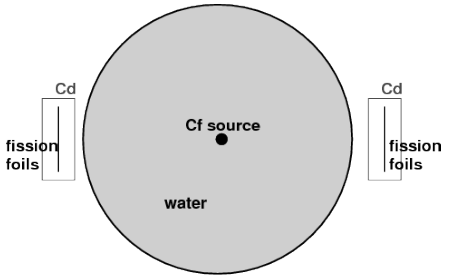
- FNS
  - ✓ Be, C, N, O, Fe, Pb
  - ✓ 5 angles



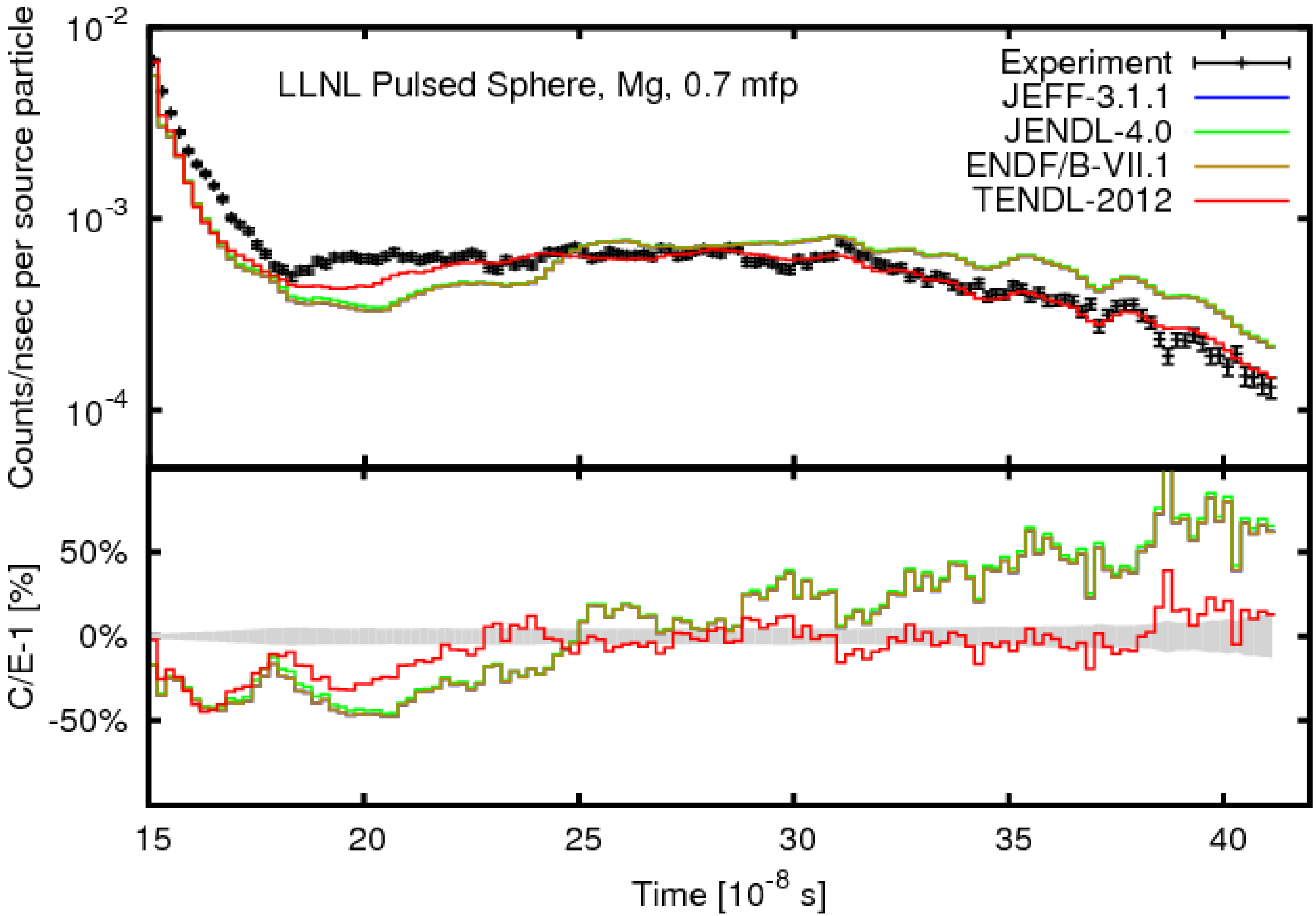
- LLNL
  - ✓ Li, Be, C, N, O, Mg, Al, Ti, Fe, Pb, D_2O, H_2O, concrete, polyethylene, teflon



- NIST
  - ✓ H_2O, Cd



Shielding example: LLNL, Mg, 0.7 mfp



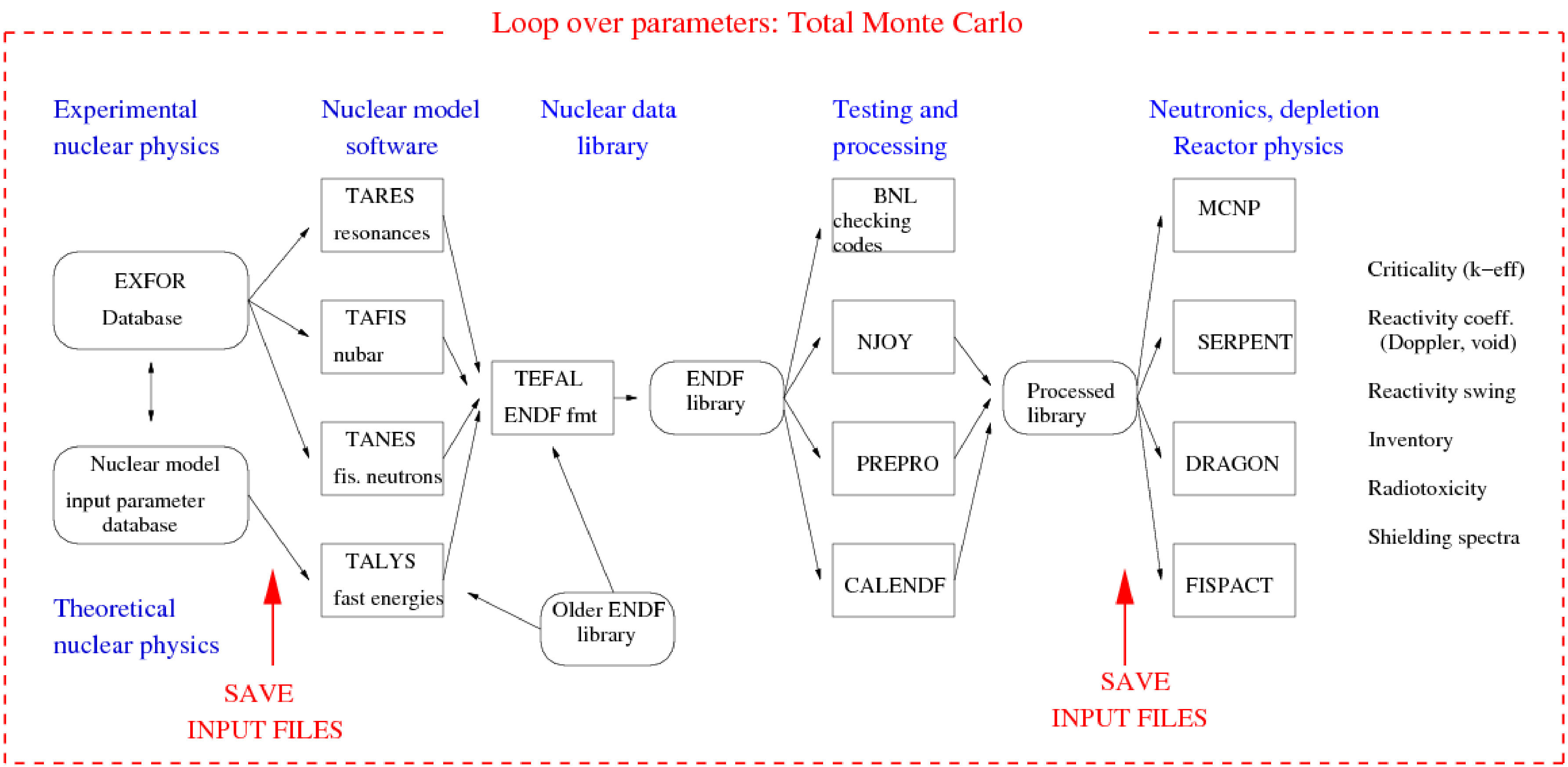
“Total” Monte Carlo

- 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)

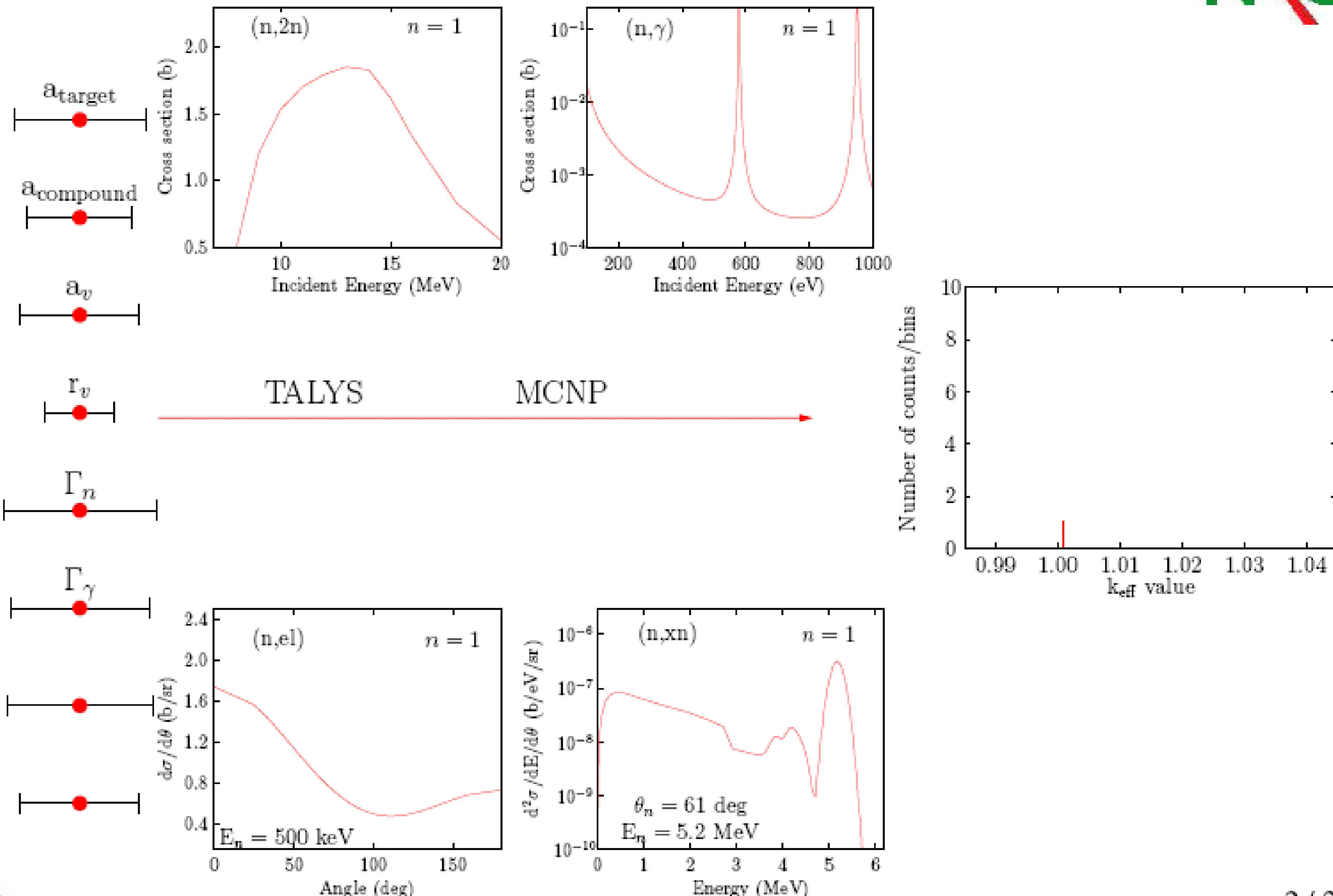
> *“Researchers should cease trying to be clever in devising refinements to old methods that were developed when computational resources were limited.*
> *Instead, their creative instincts should be redirected to unleashing the full potential of computers for* **brute** *force analysis”*

D. Smith, Santa Fe 2004

Automating nuclear reactions: Total Monte Carlo



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



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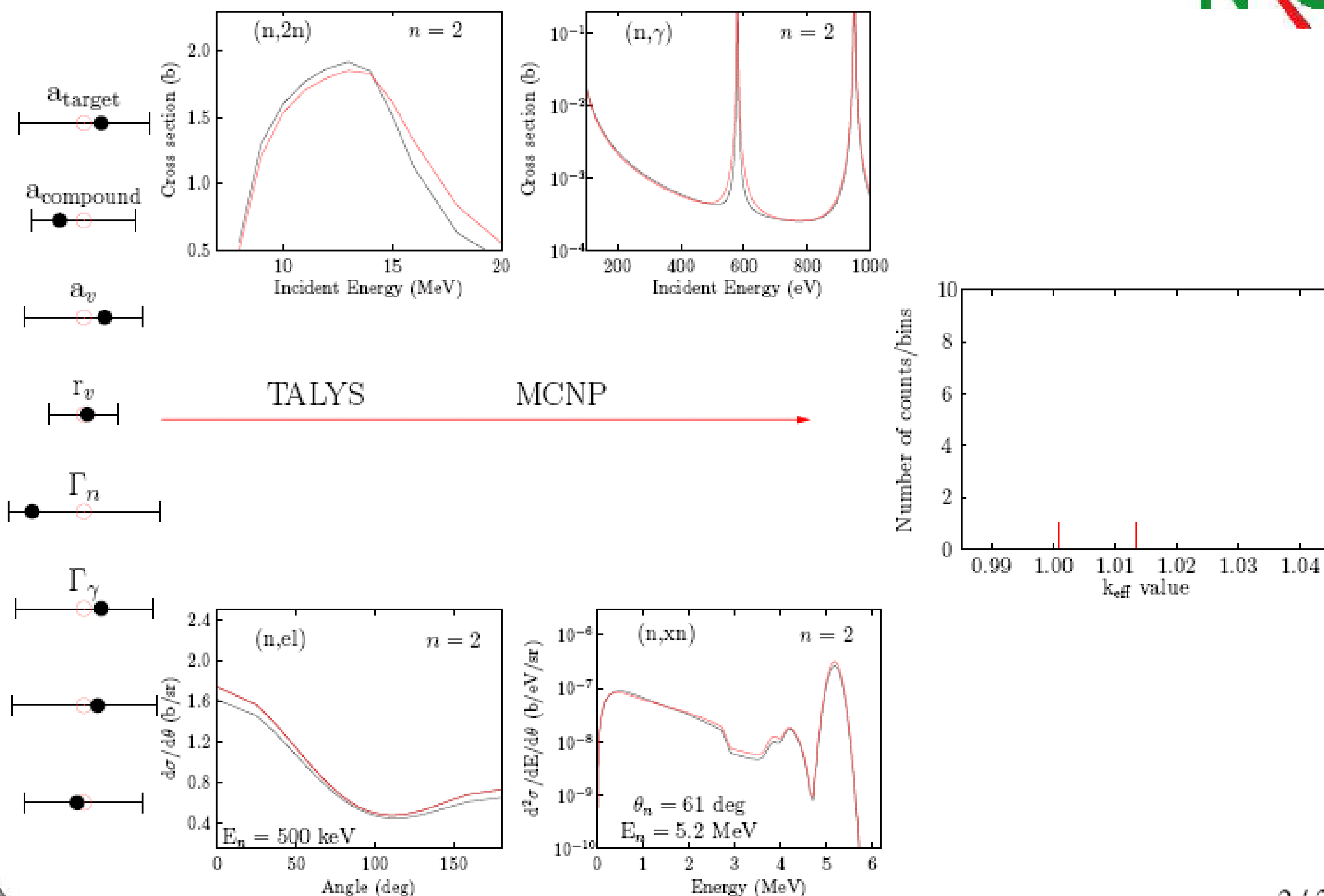

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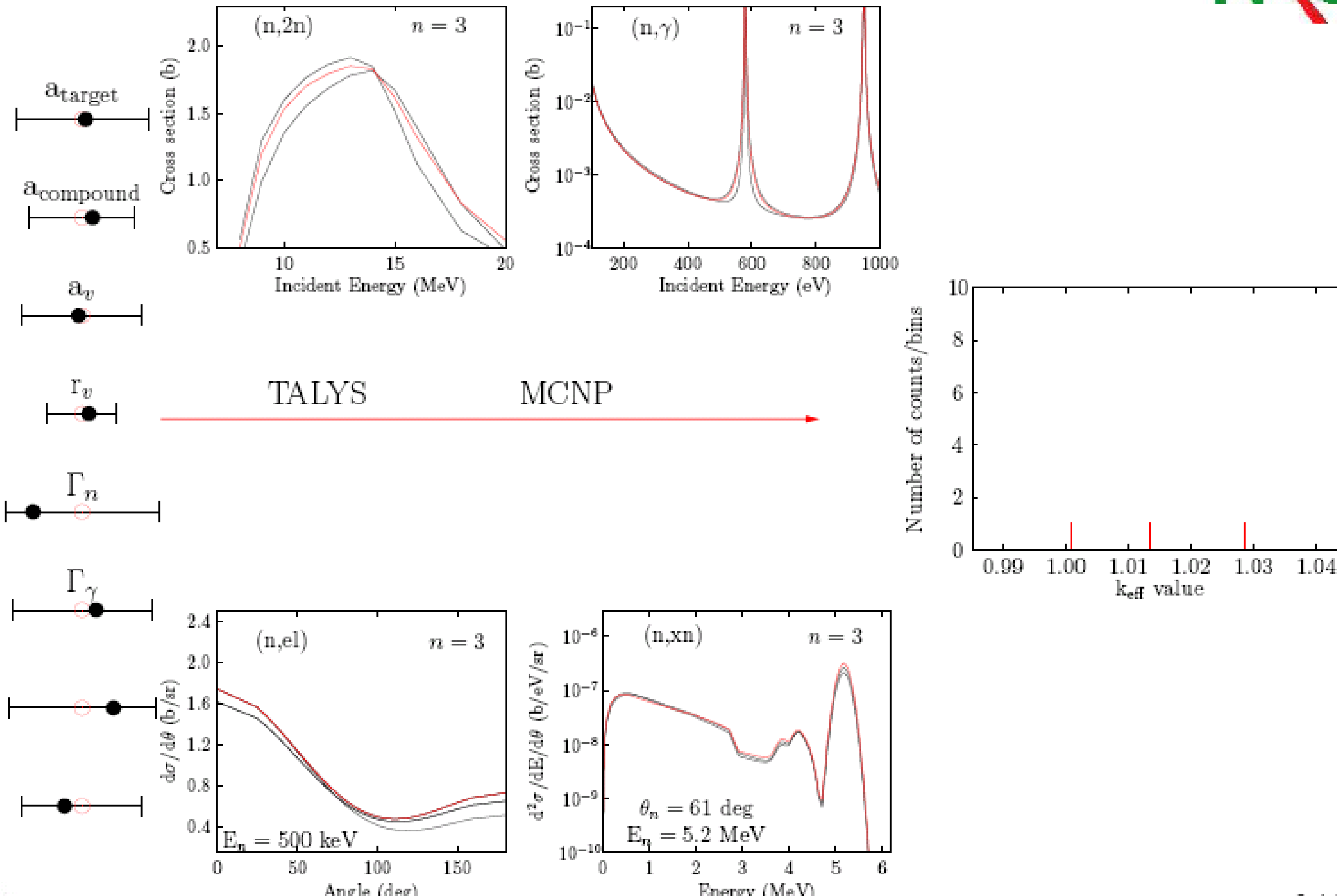

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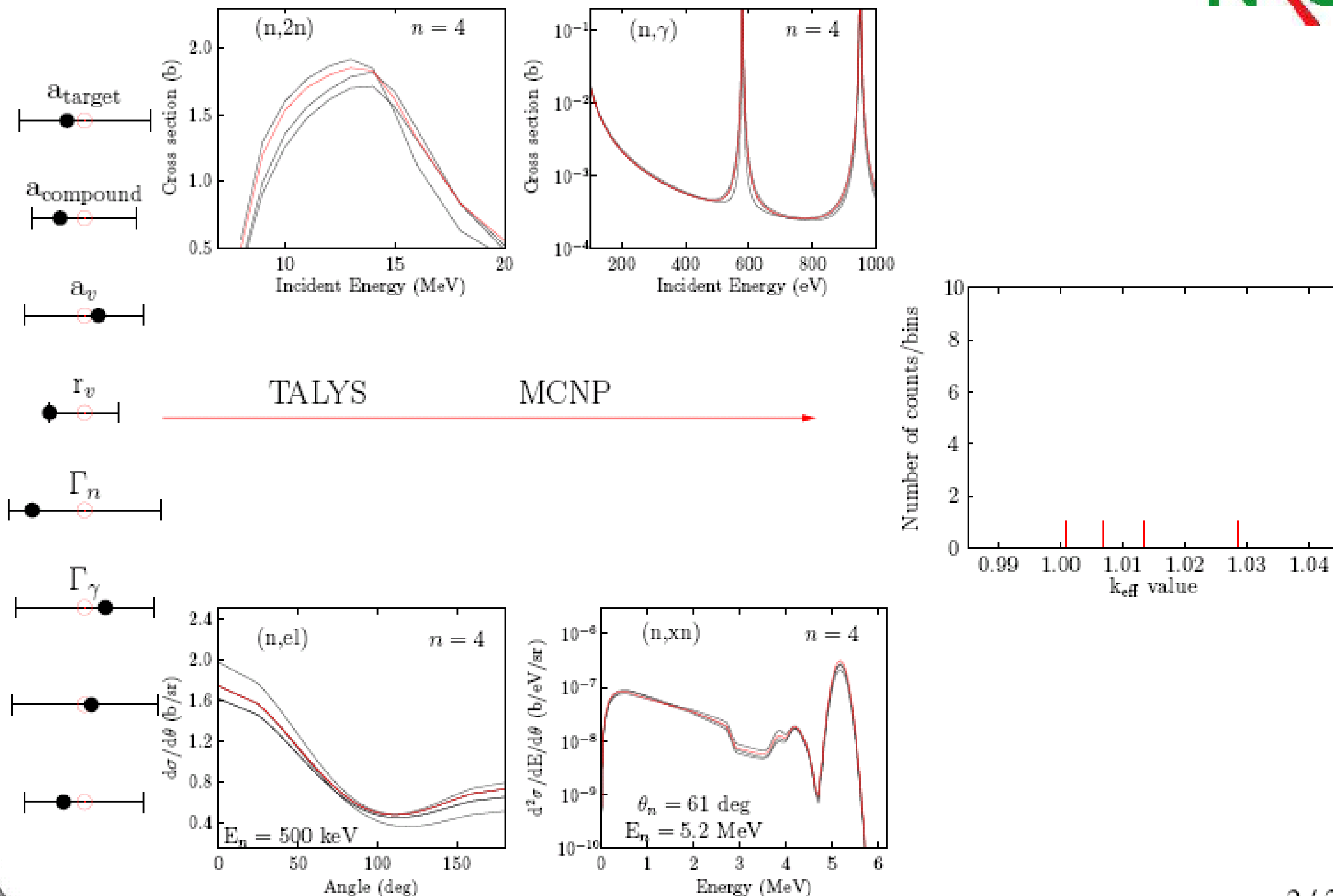

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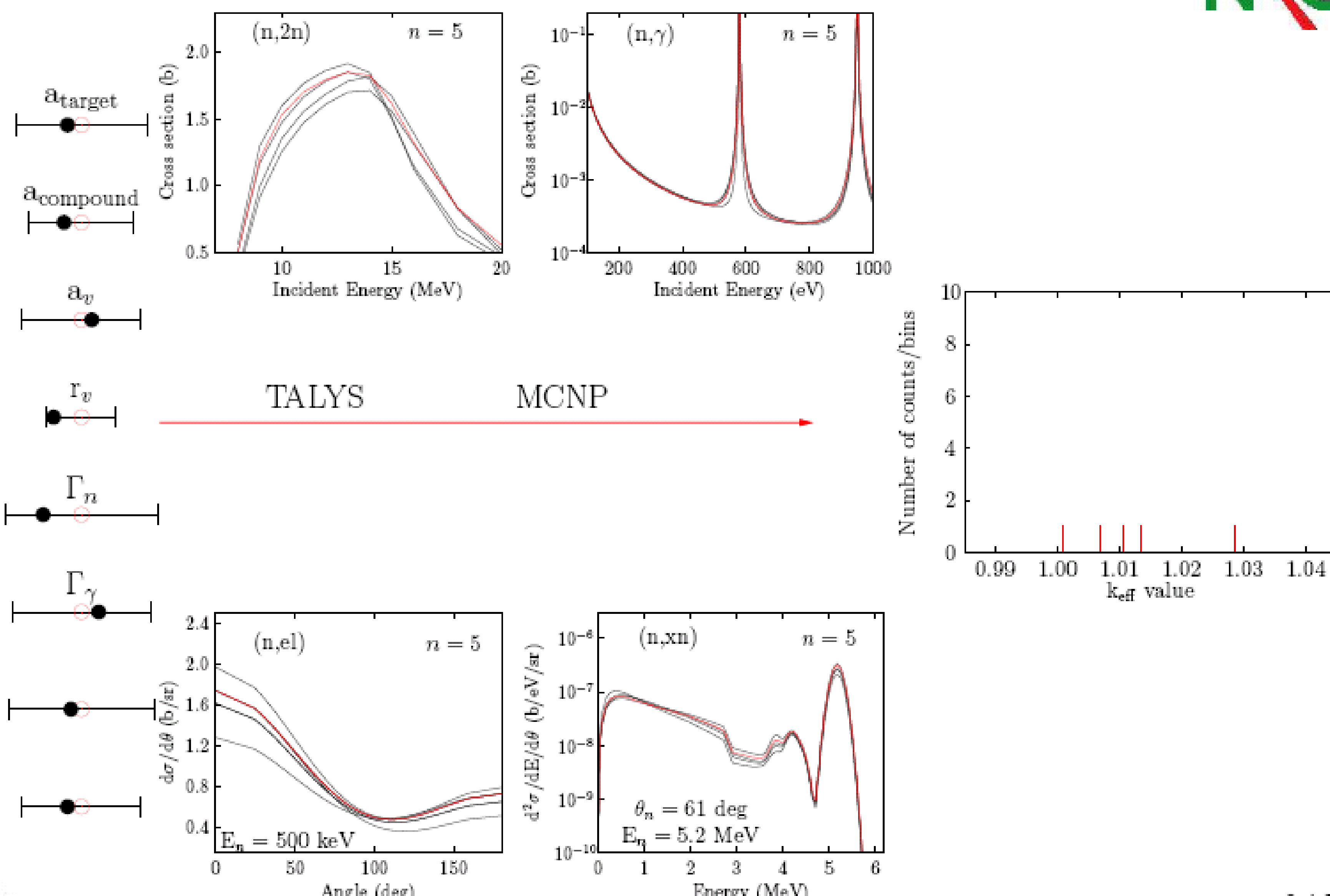

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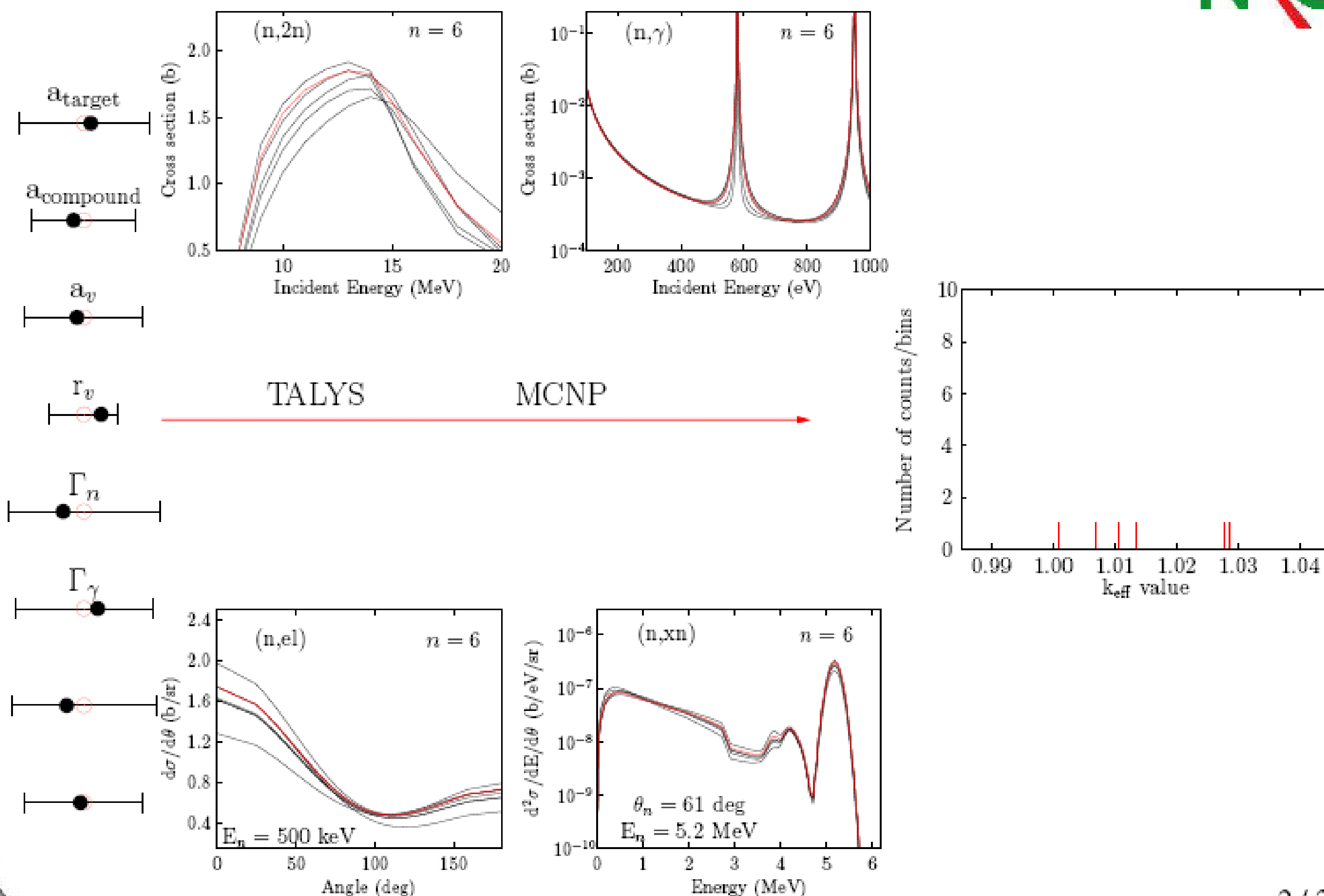

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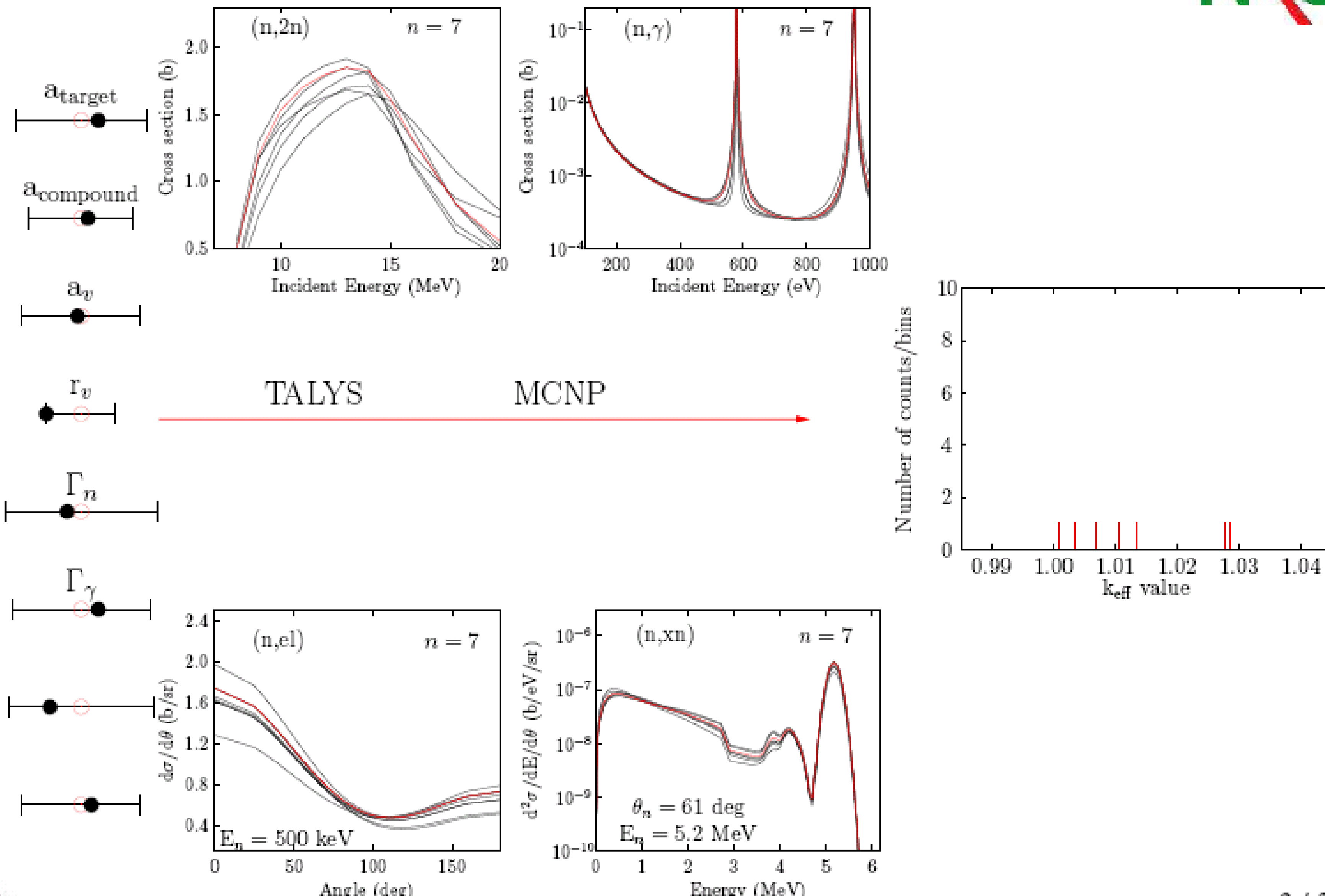

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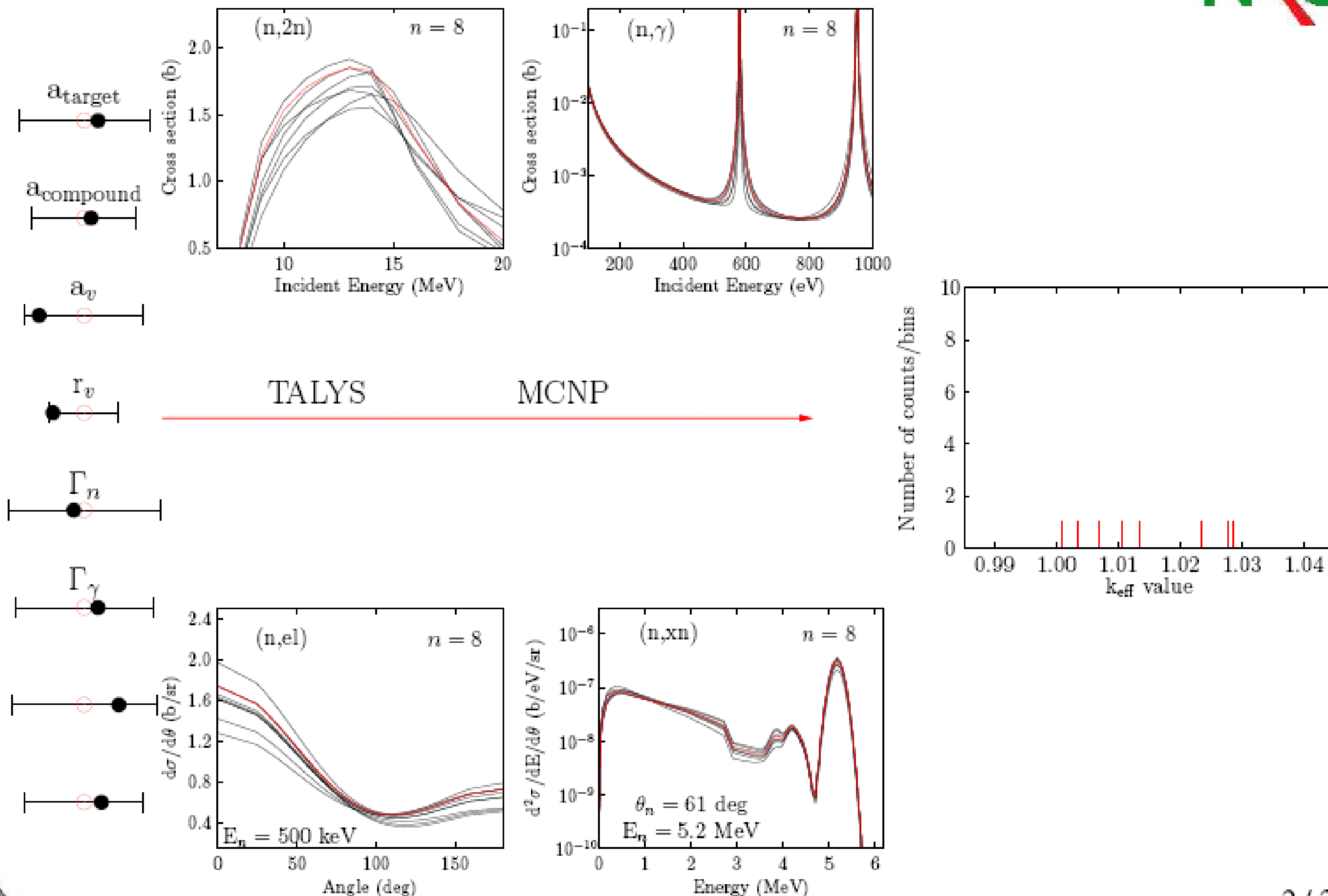

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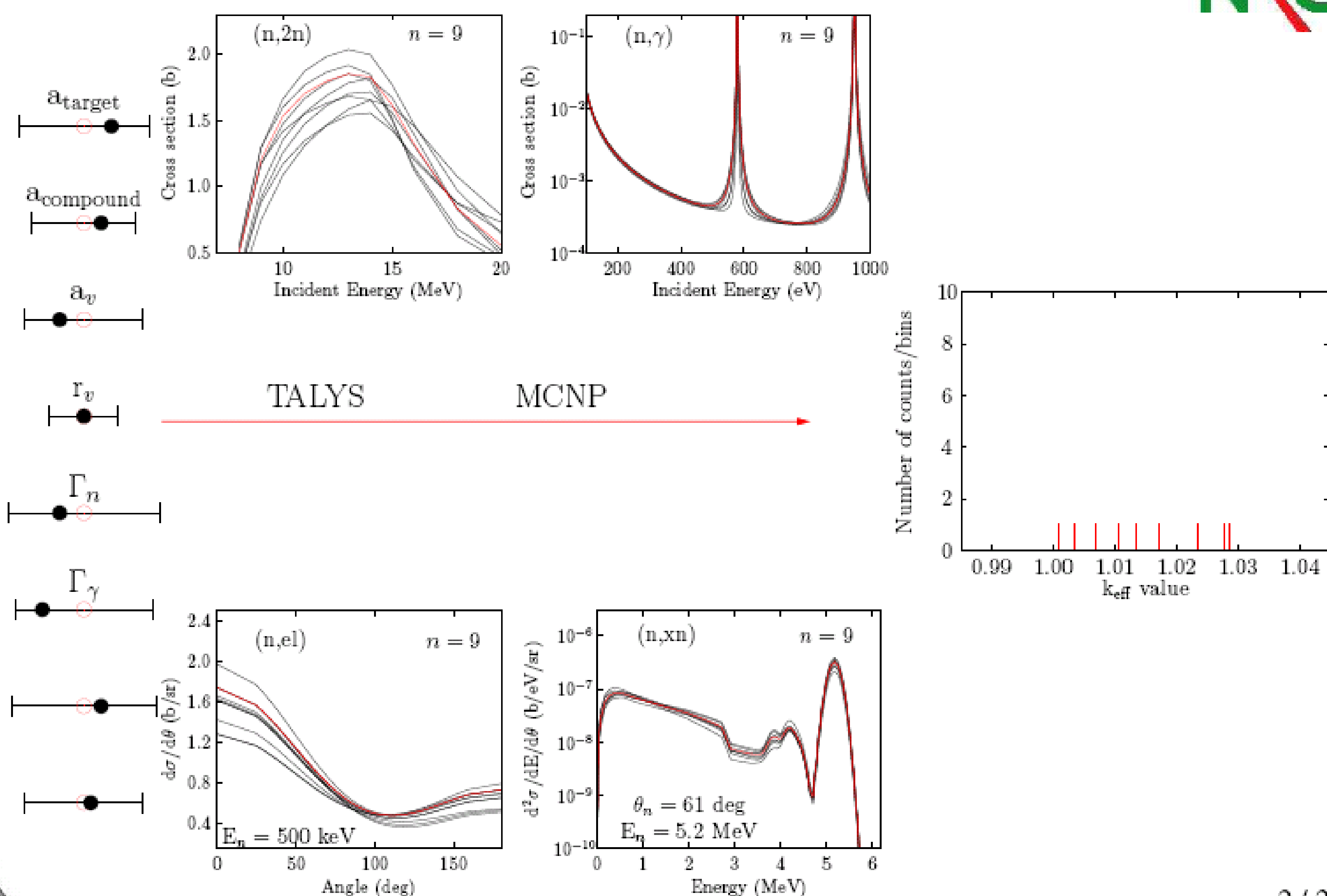

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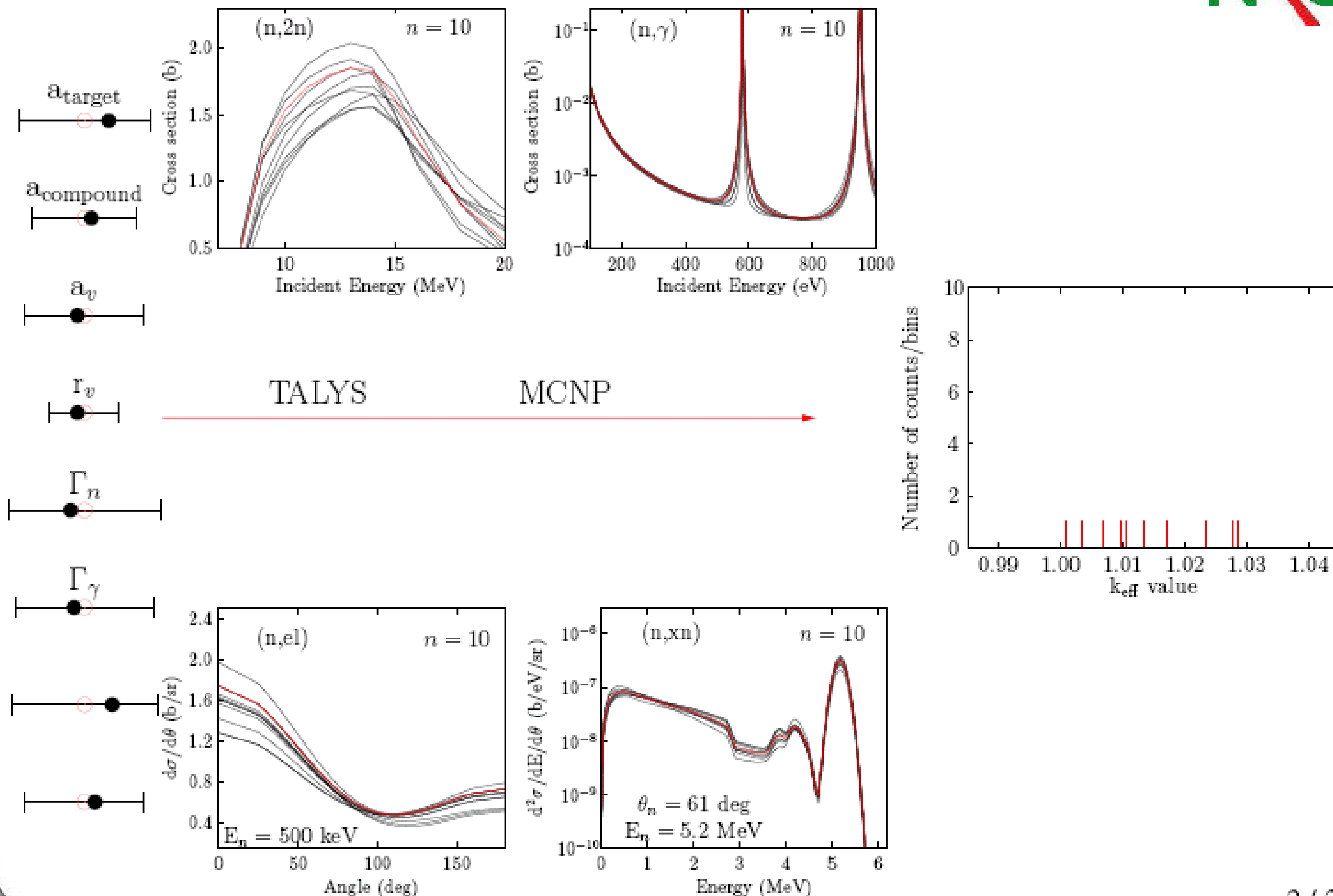

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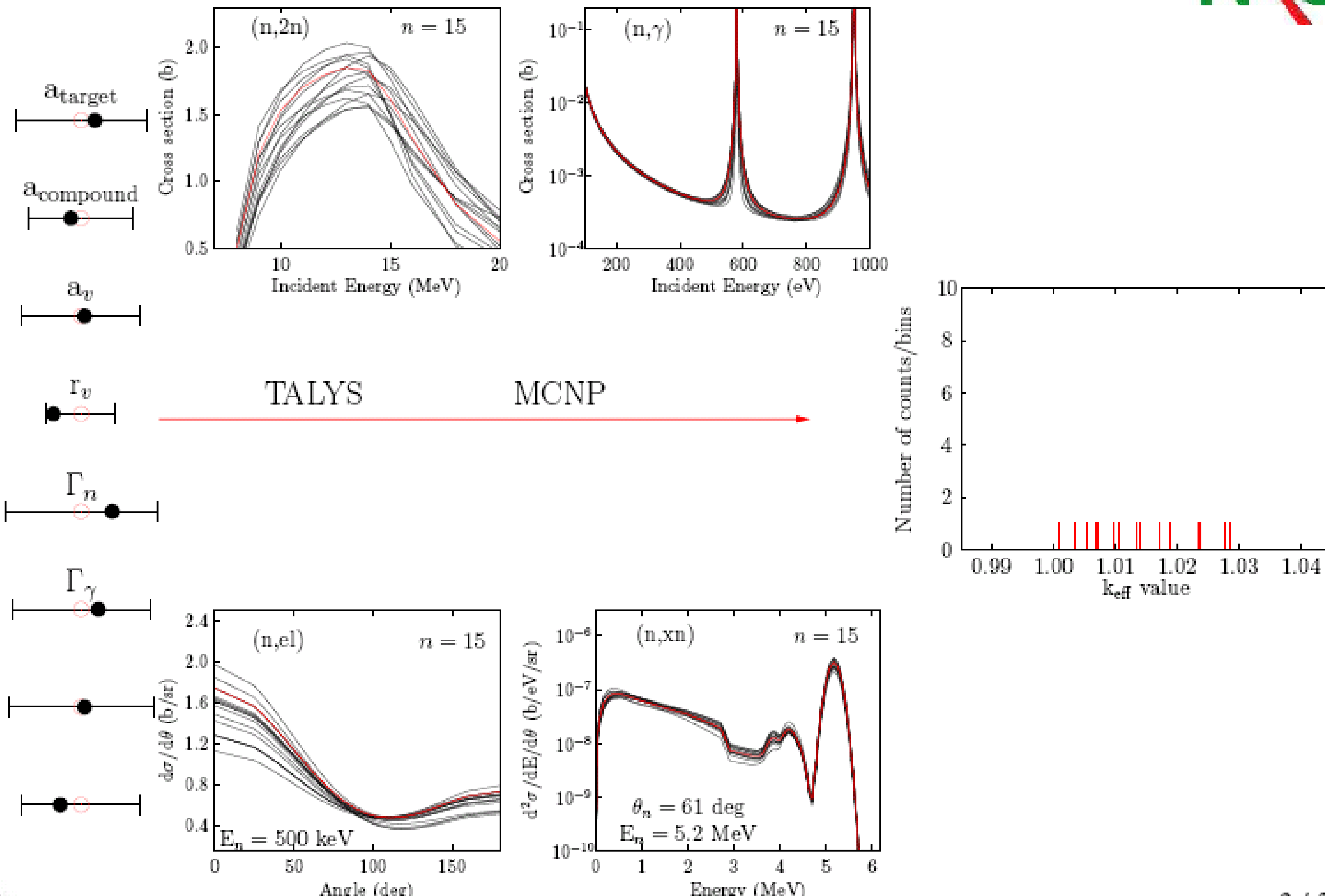

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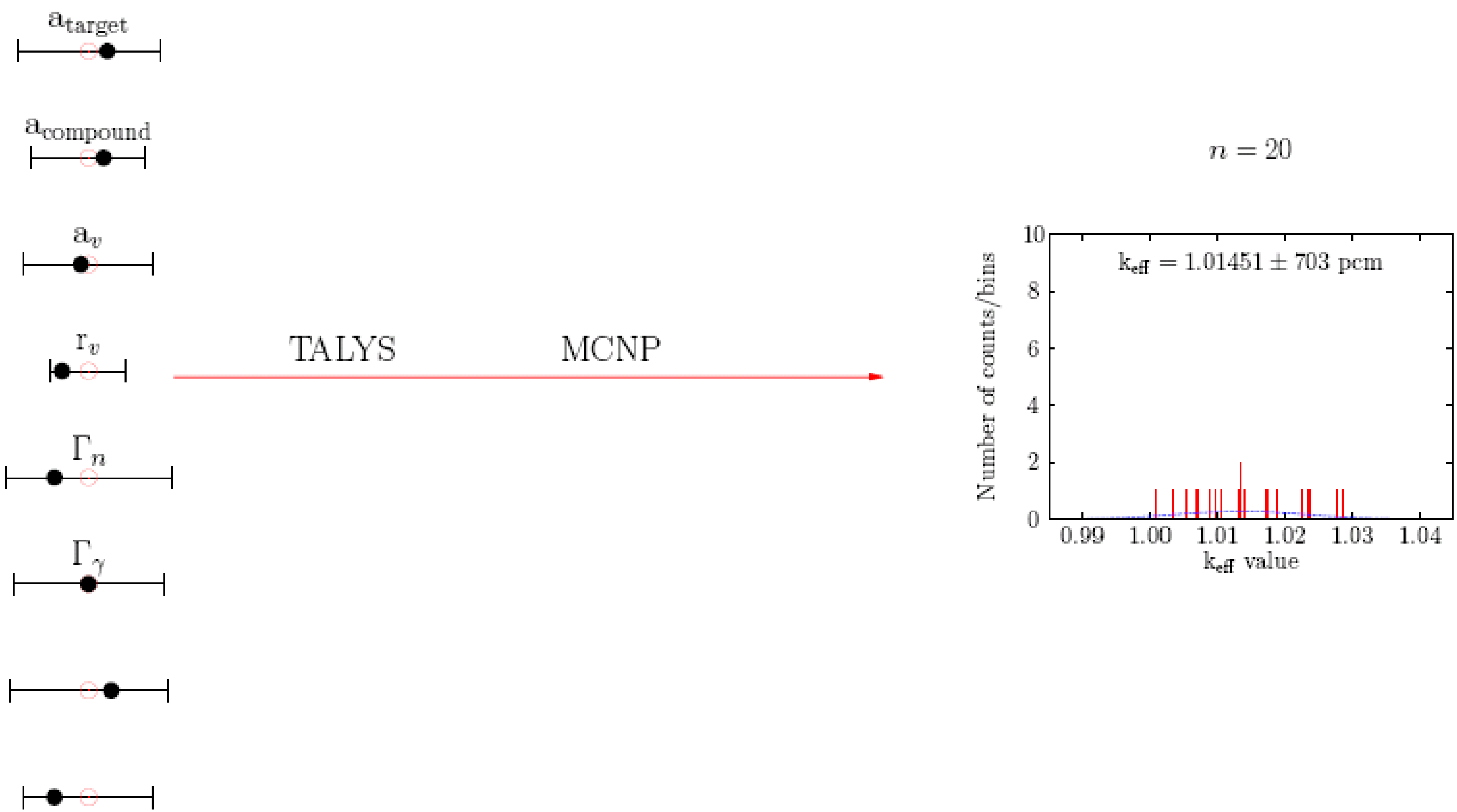

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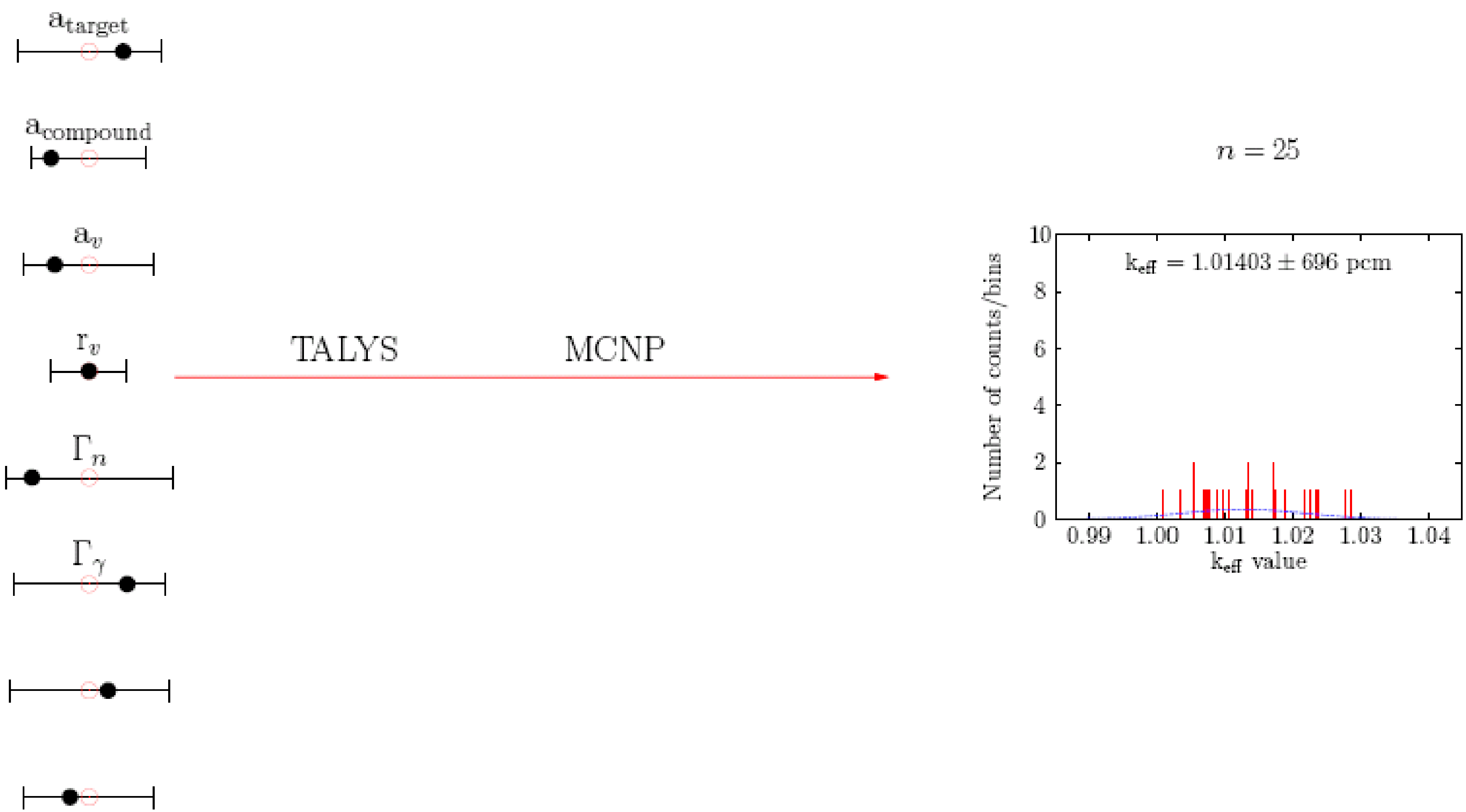

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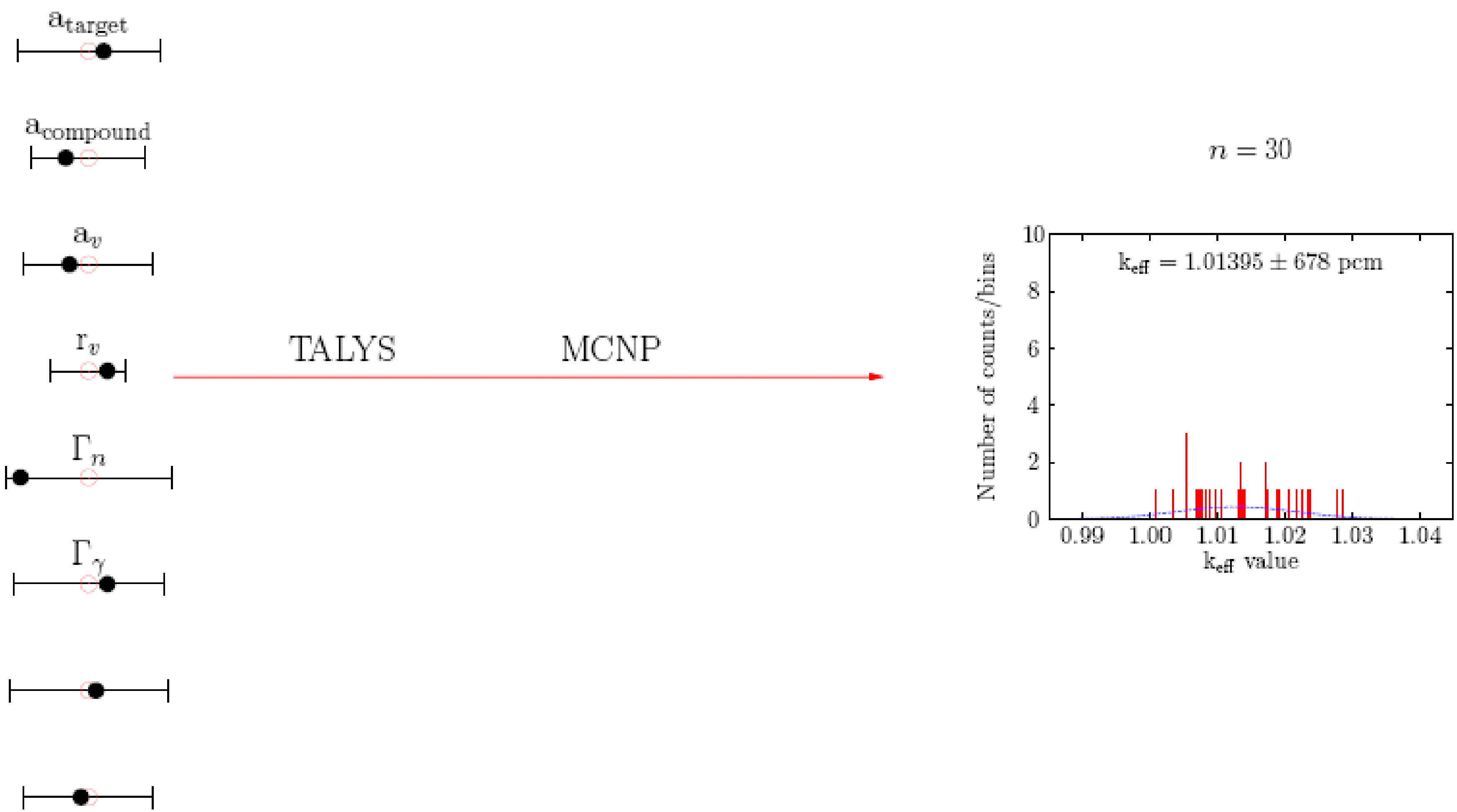

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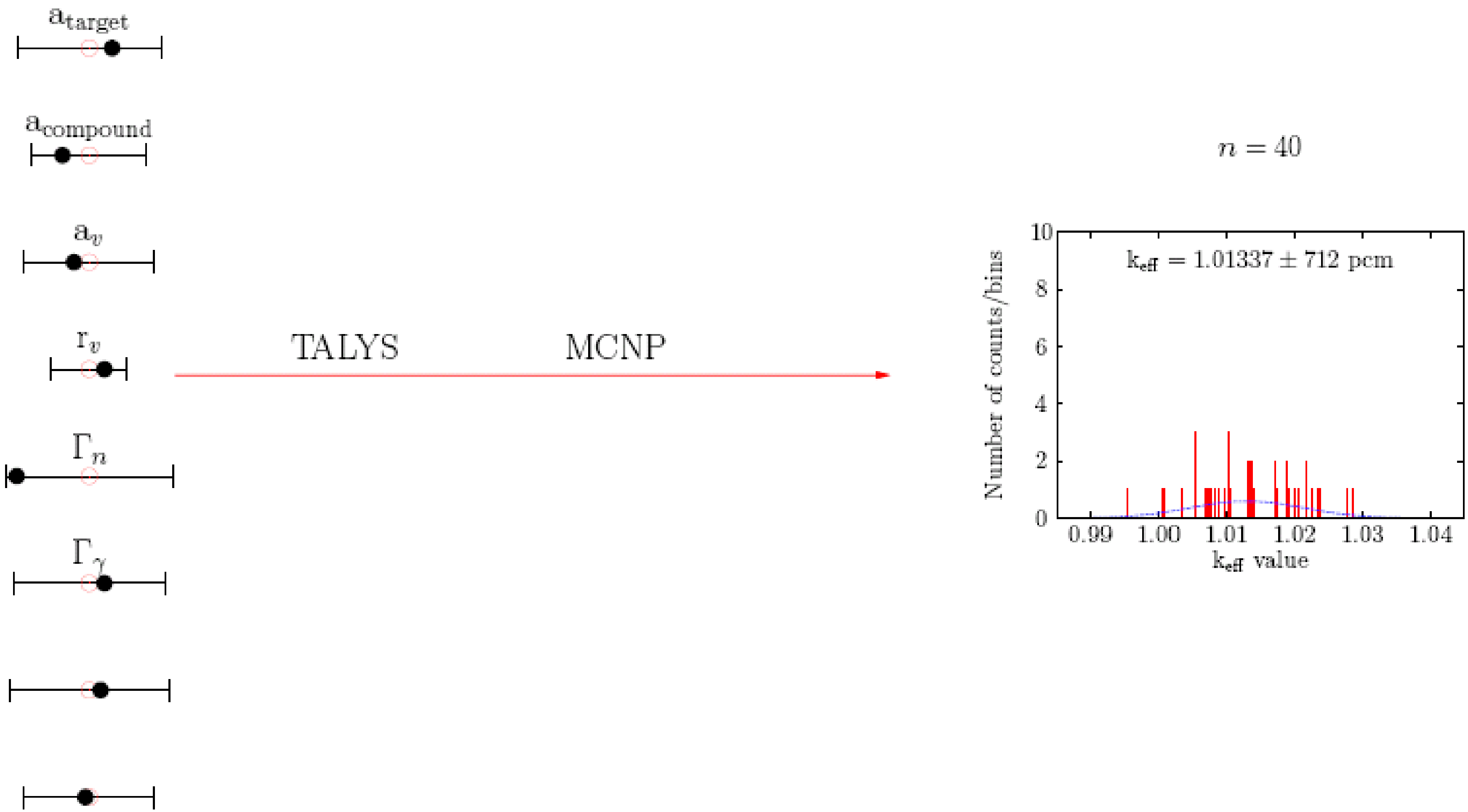

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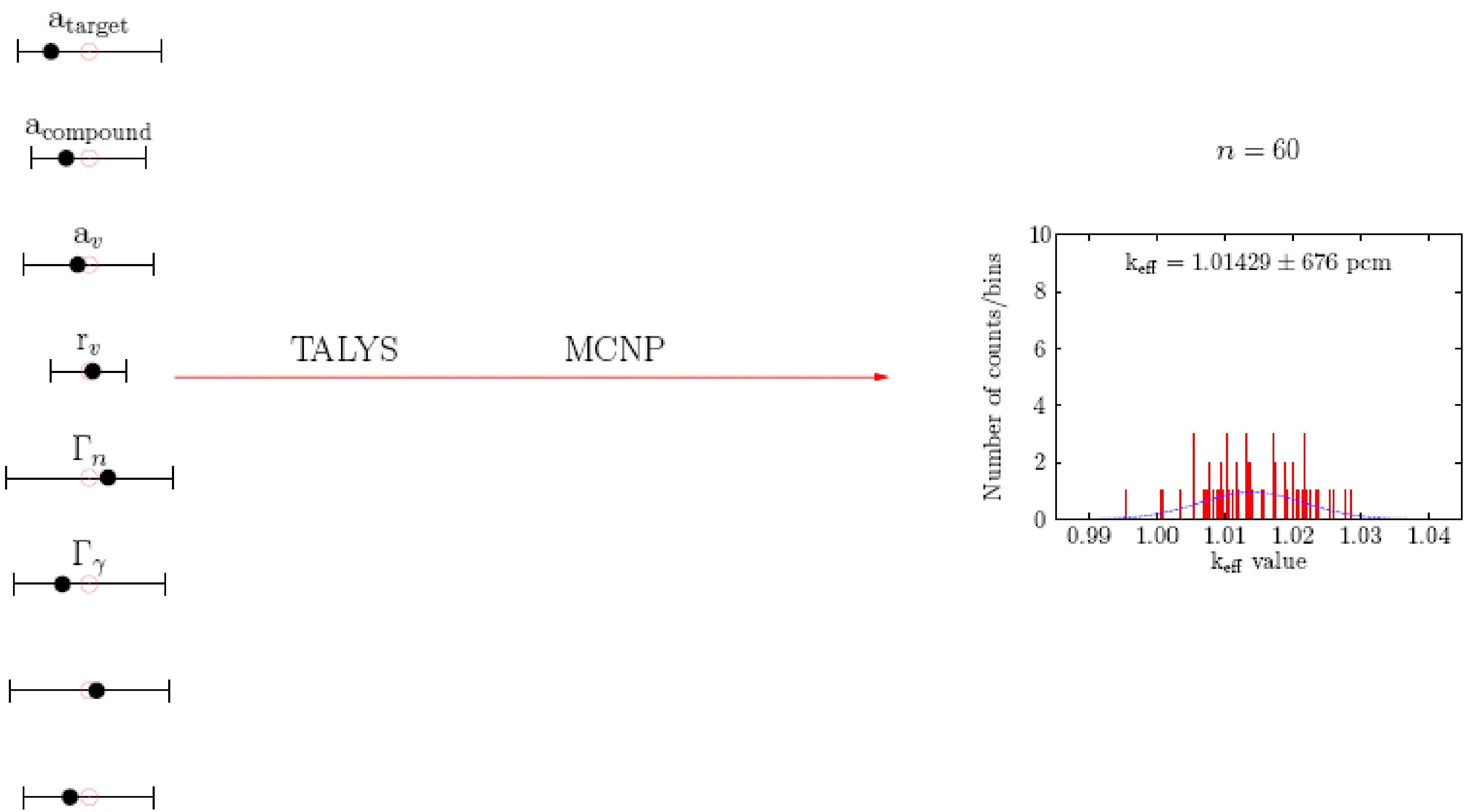

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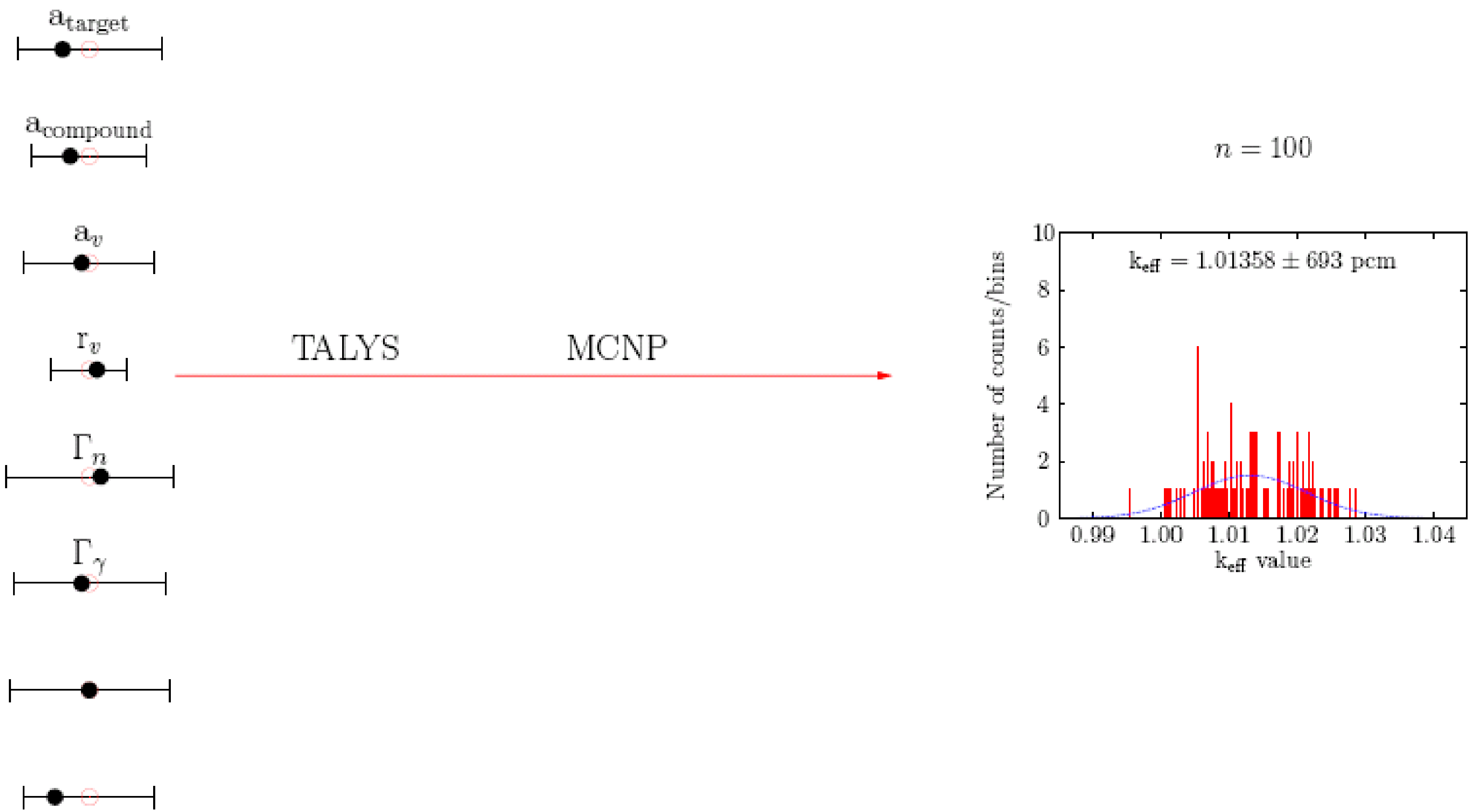

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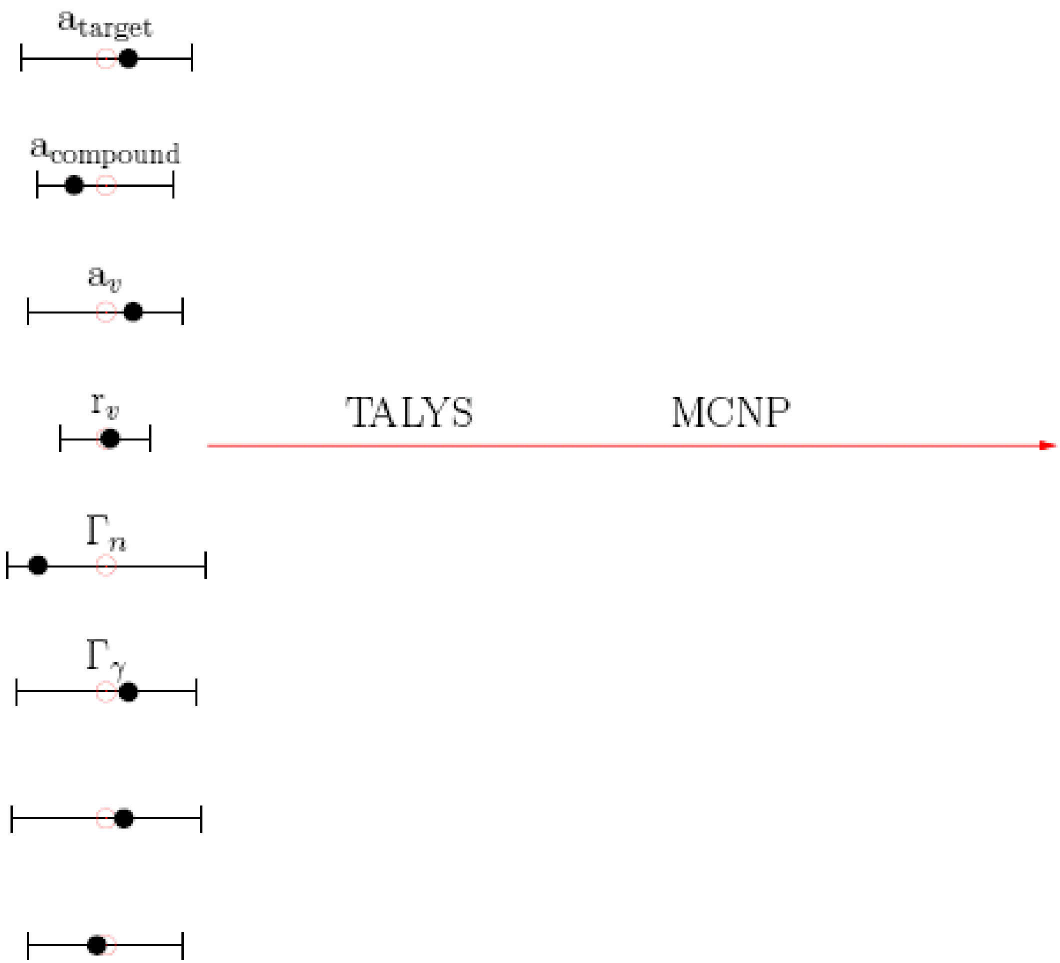
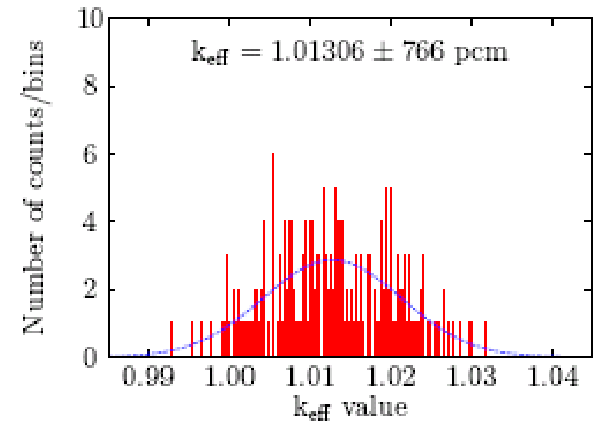


$n = 200$



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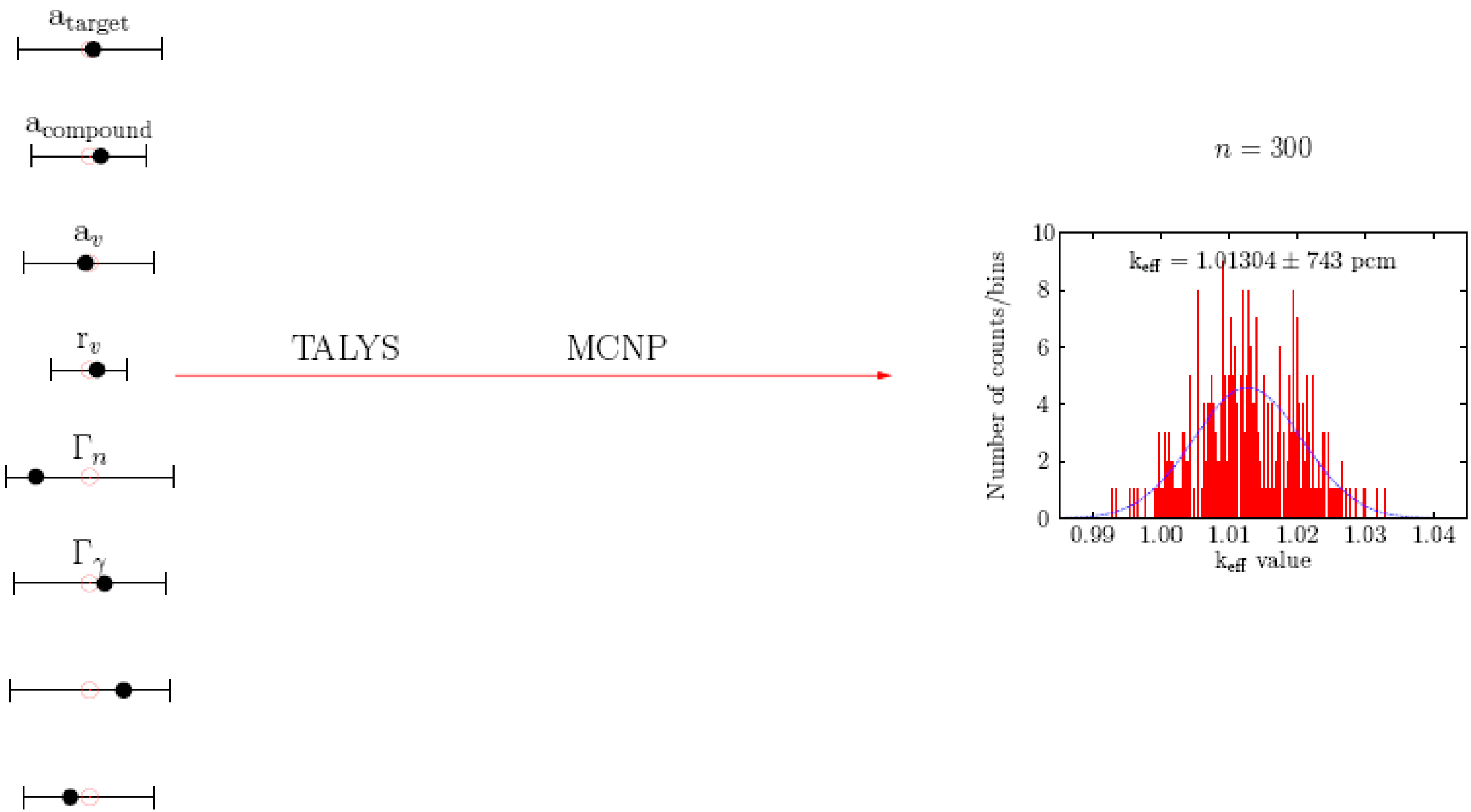

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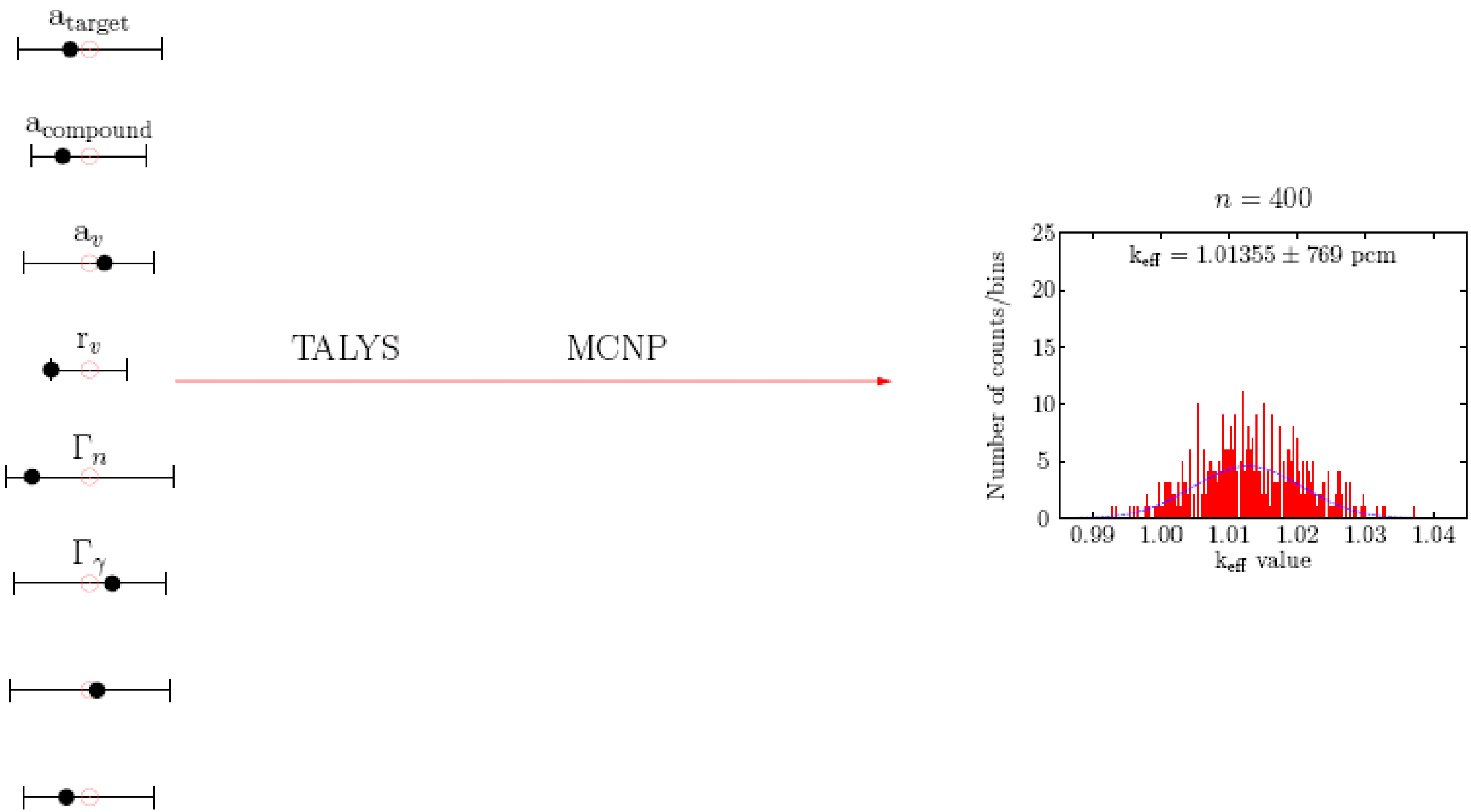

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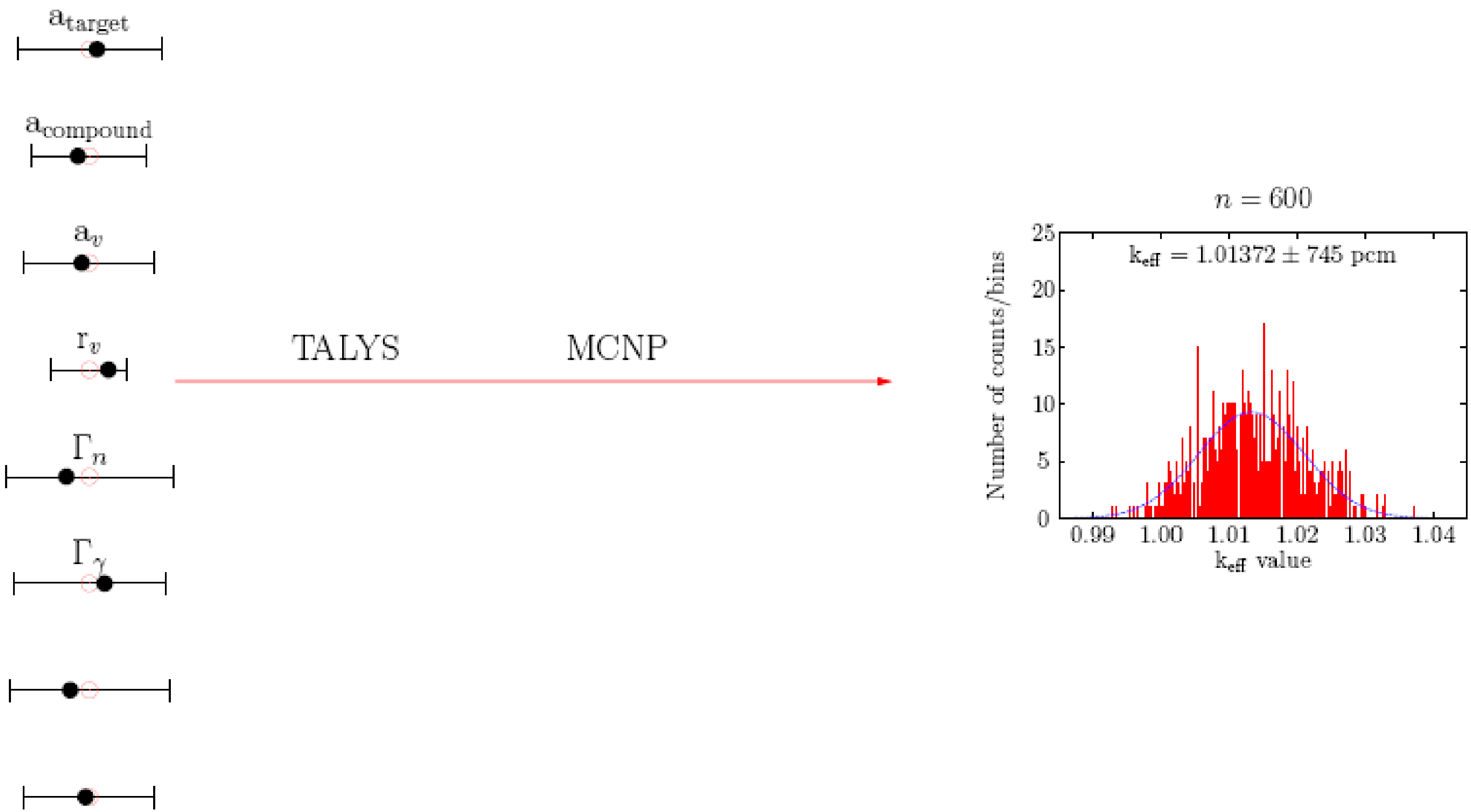

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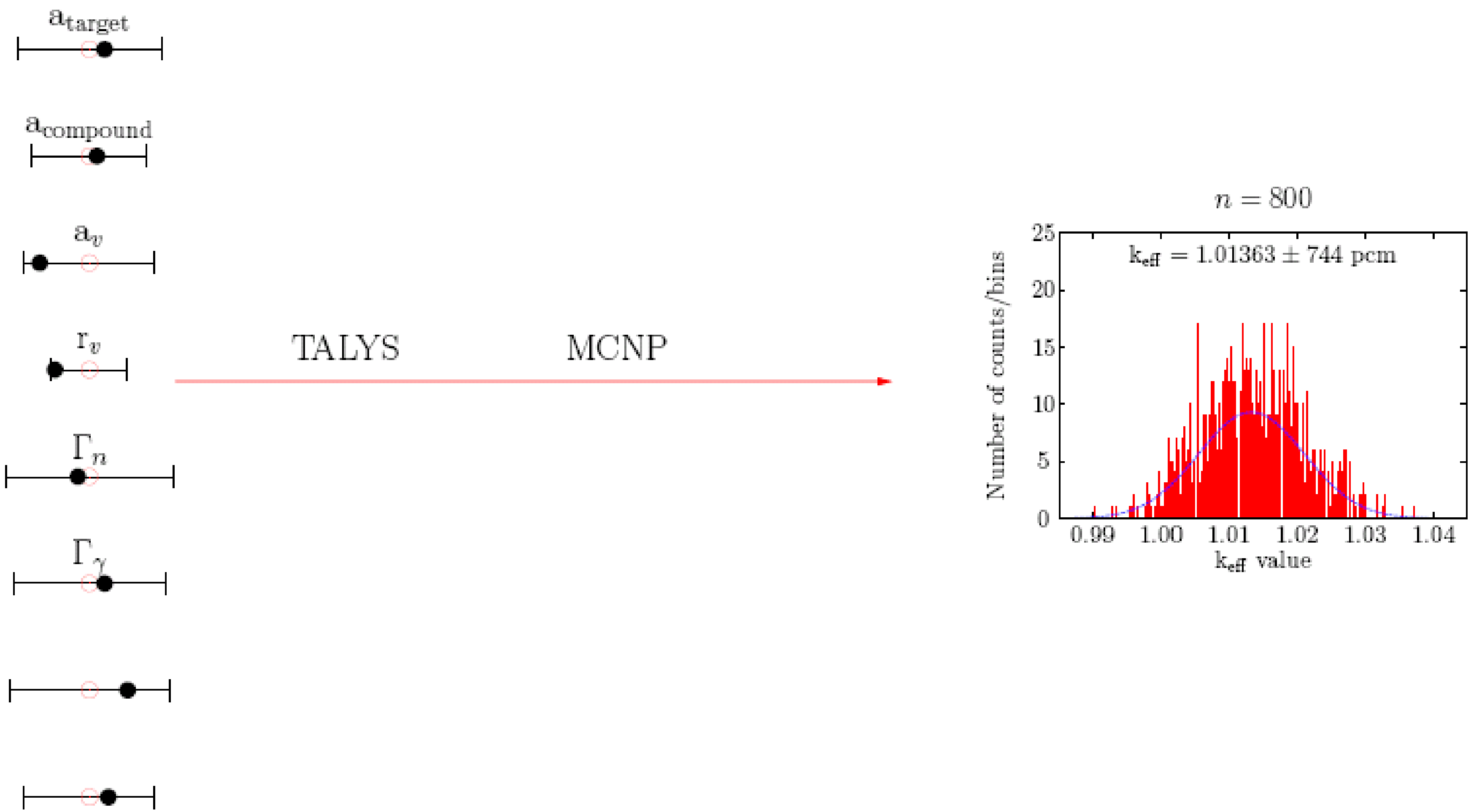

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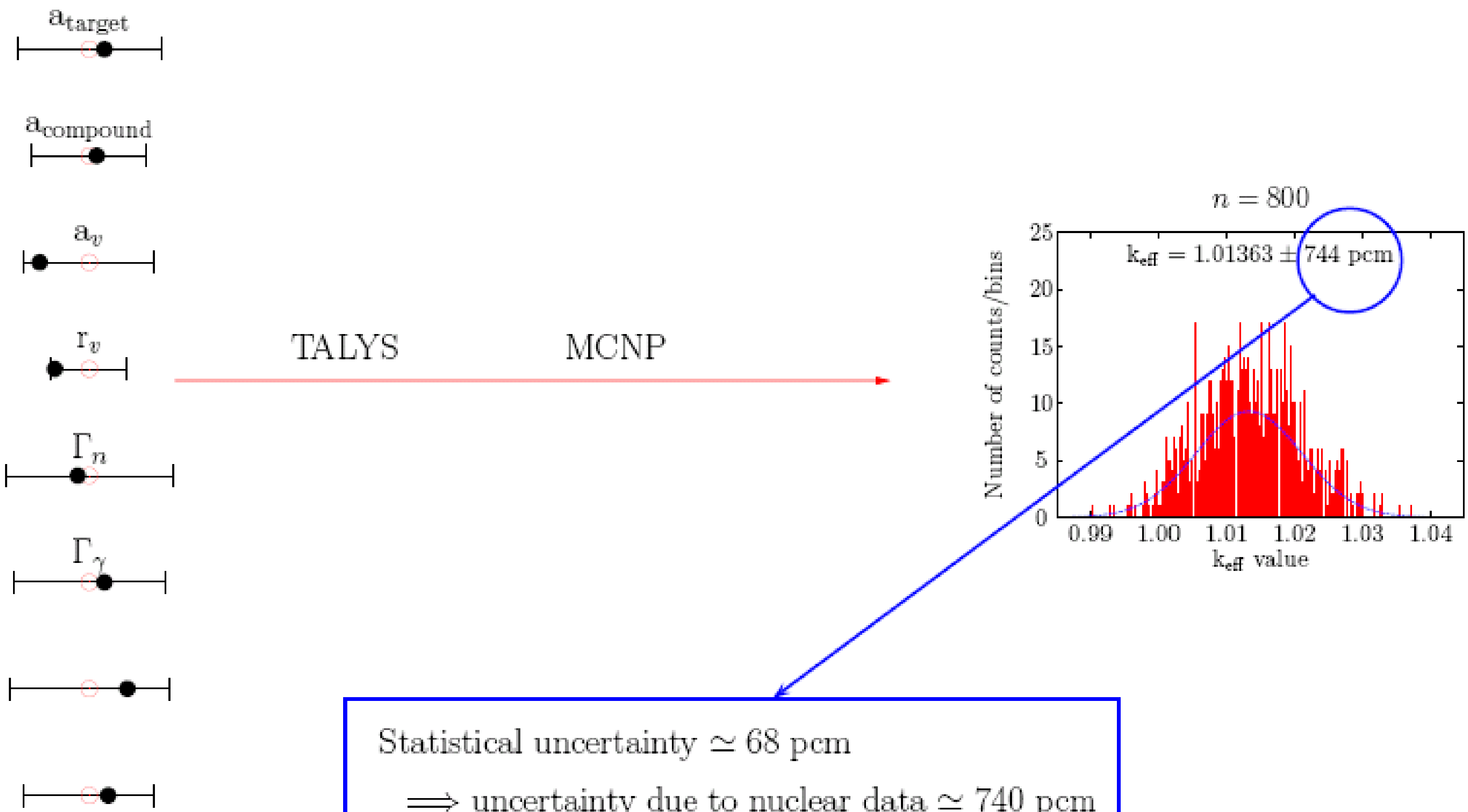


Statistical uncertainty $\simeq$ 68 pcm

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

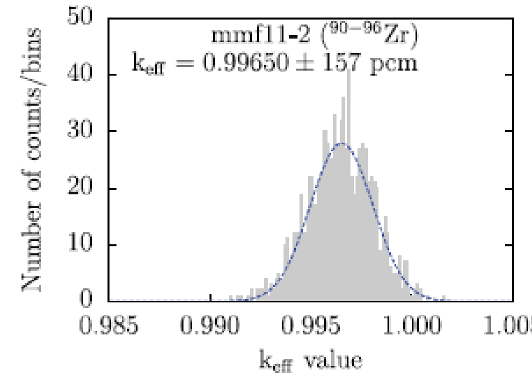
TMC Application: criticality benchmarks

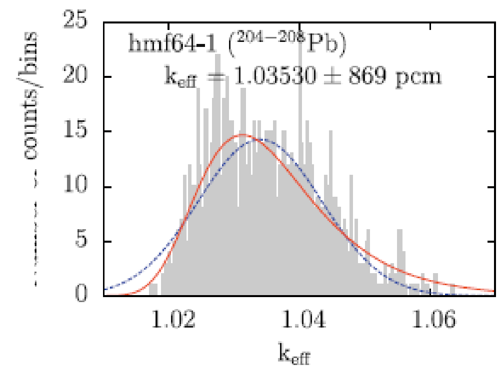
Total of 60000 random ENDF-6 files

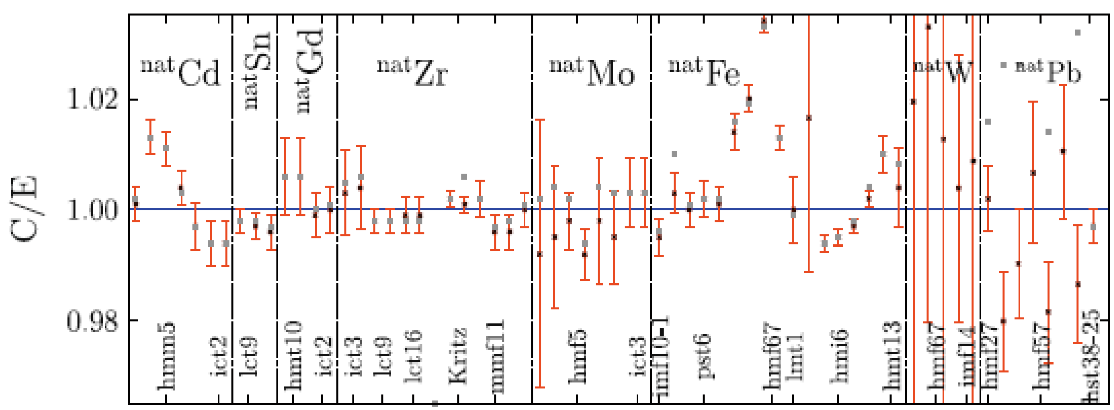
Sometimes deviation from Gaussian shape

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).

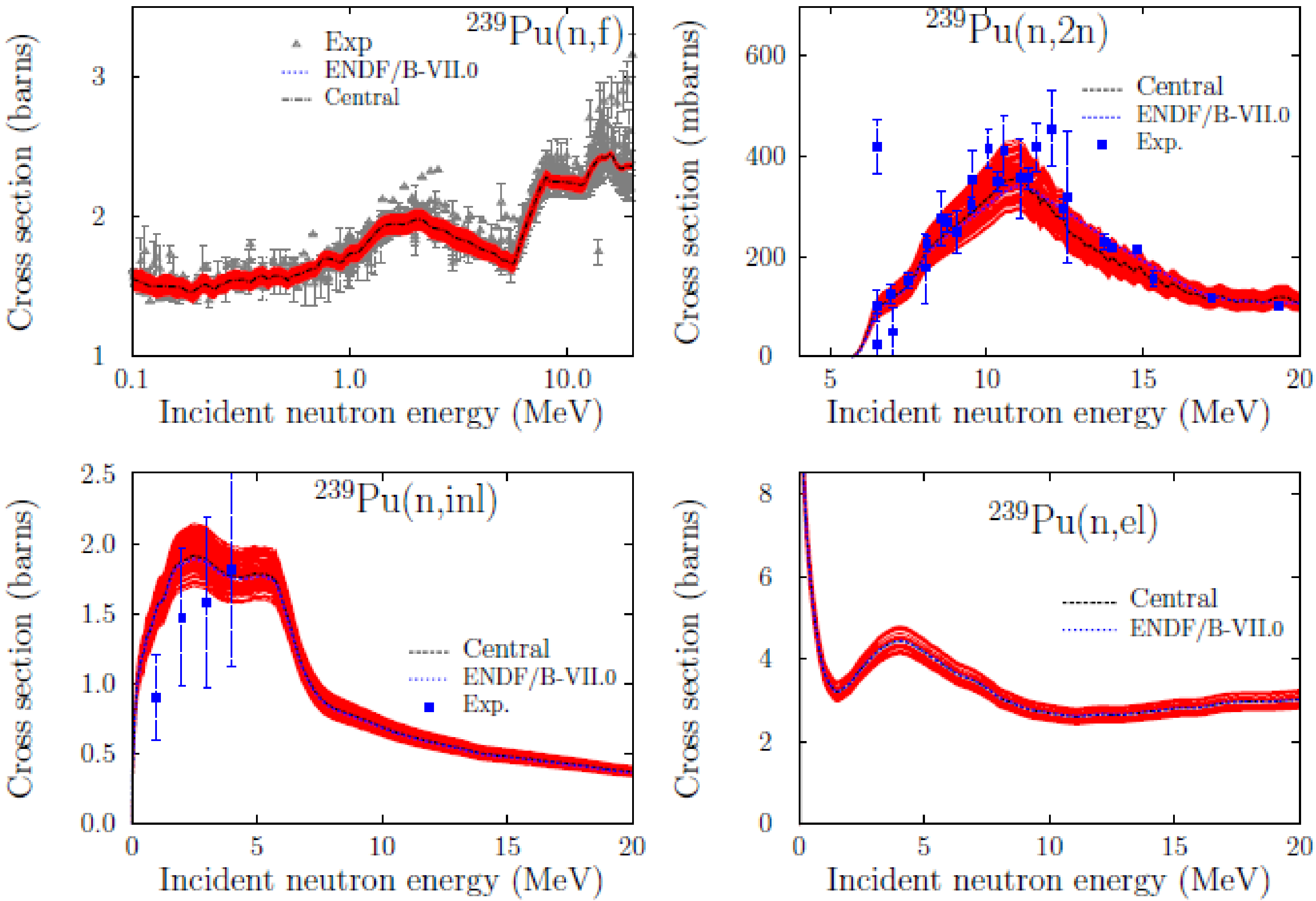
Yields uncertainties on benchmarks !







Pu239 cross sections + uncertainties

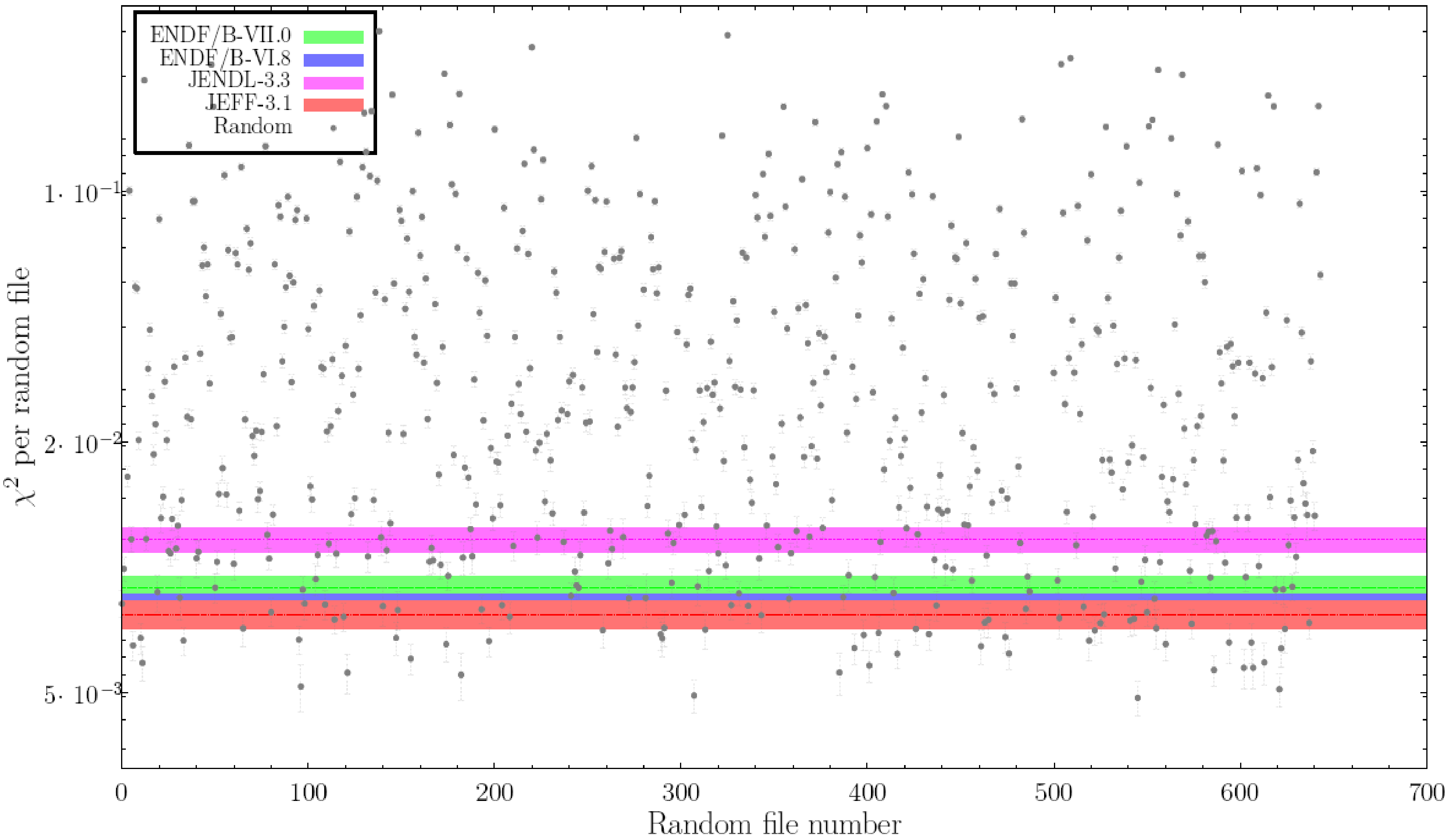


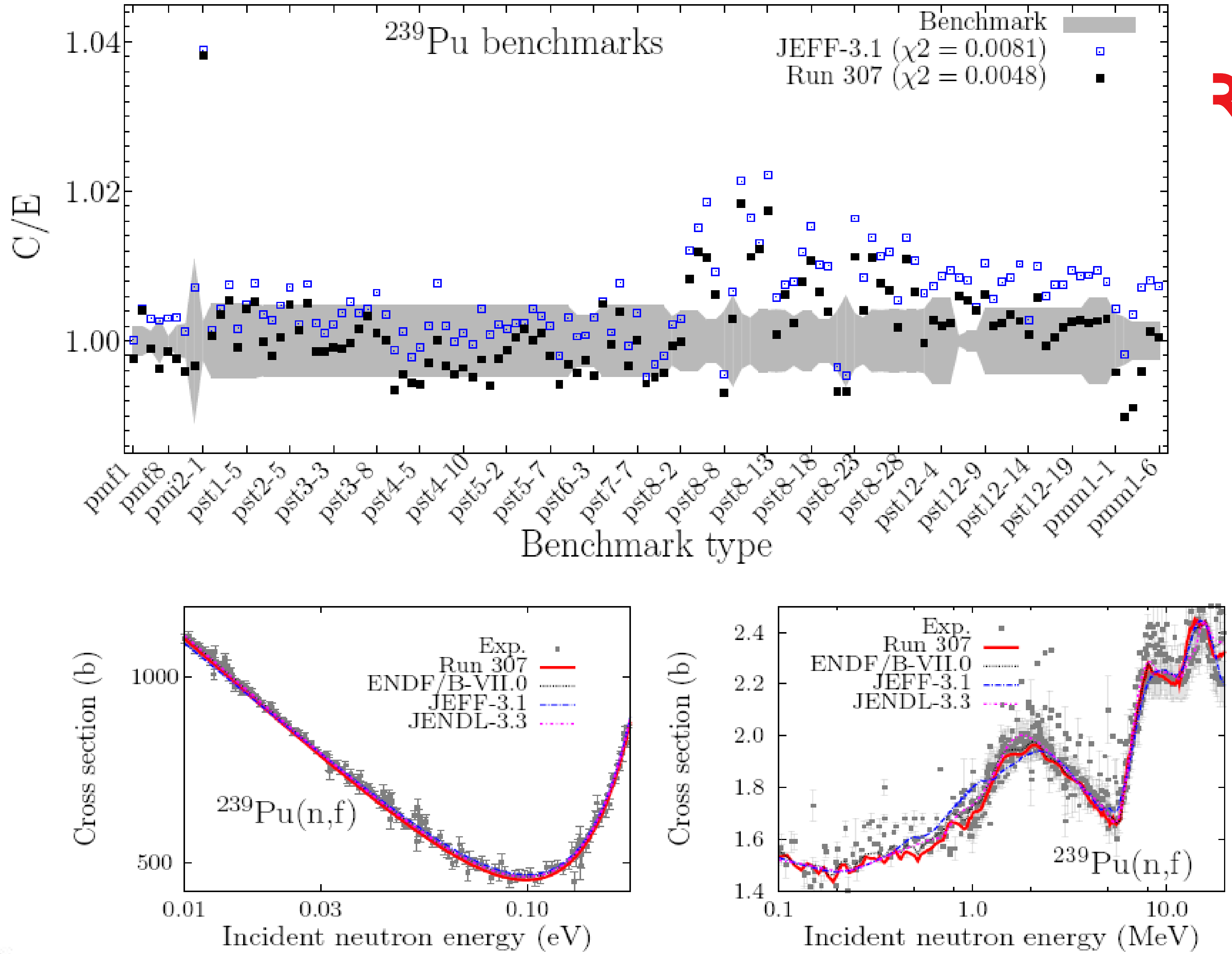
Optimization of Pu-239

- Select 120 ICSBEP benchmarks
- Create 630 random Pu-239 libraries, all within, or closely around, the uncertainty bands
- Do a total of 120 x 630 =75600 MCNP criticality calculations
- Do another 120 x 4 calculations:

  - for JEFF-3.1, $\chi^2 = 8.08e^{-3} +/- 7.2e^{-4}$
  - for ENDF/B-VII.0, $\chi^2 = 9.55e^{-3} +/- 7.9e^{-4}$
  - for ENDF/B-VI.8, $\chi^2 = 8.45e^{-3} +/- 7.2e^{-4}$
  - for JENDL-3.3, $\chi^2 = 1.31e^{-2} +/- 1.0e^{-3}$

Optimization of Pu-239

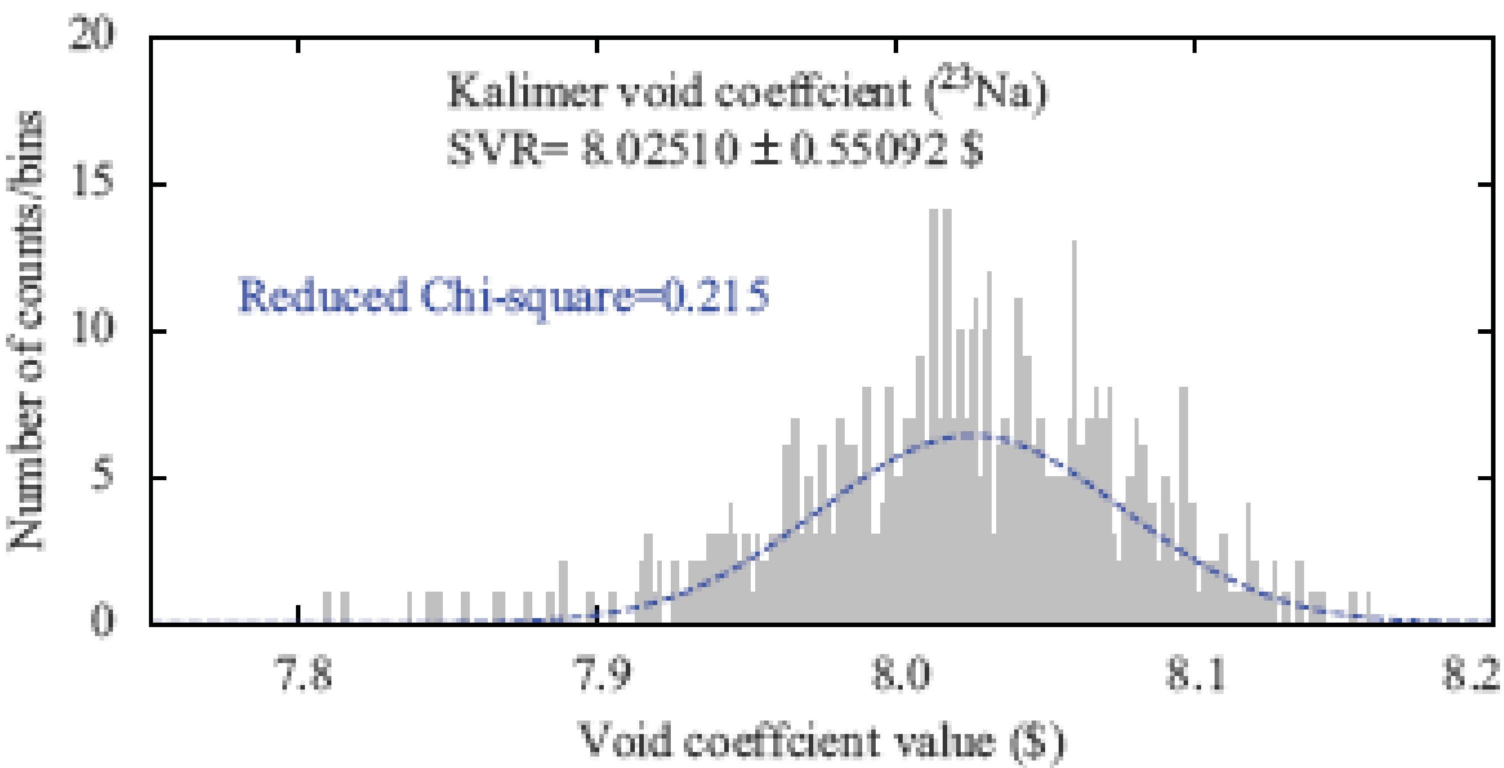




²³⁹Pu benchmarks
Benchmark
JEFF-3.1 (χ2 = 0.0081)
Run 307 (χ2 = 0.0048)
C/E
1.04
1.02
1.00
pmf1
pmf8
pmi2-1
pst1-5
pst2-5
pst3-3
pst3-8
pst4-5
pst4-10
pst5-2
pst5-7
pst6-3
pst7-7
pst8-2
pst8-8
pst8-13
pst8-18
pst8-23
pst8-28
pst12-4
pst12-9
pst12-14
pst12-19
pmm1-1
pmm1-6
Benchmark type
Exp.
Run 307
ENDF/B-VII.0
JEFF-3.1
JENDL-3.3
Cross section (b)
1000
500
²³⁹Pu(n,f)
0.01
0.03
0.10
Incident neutron energy (eV)
Exp.
Run 307
ENDF/B-VII.0
JEFF-3.1
JENDL-3.3
Cross section (b)
2.4
2.2
2.0
1.8
1.6
1.4
0.1
1.0
10.0
²³⁹Pu(n,f)
Incident neutron energy (MeV)

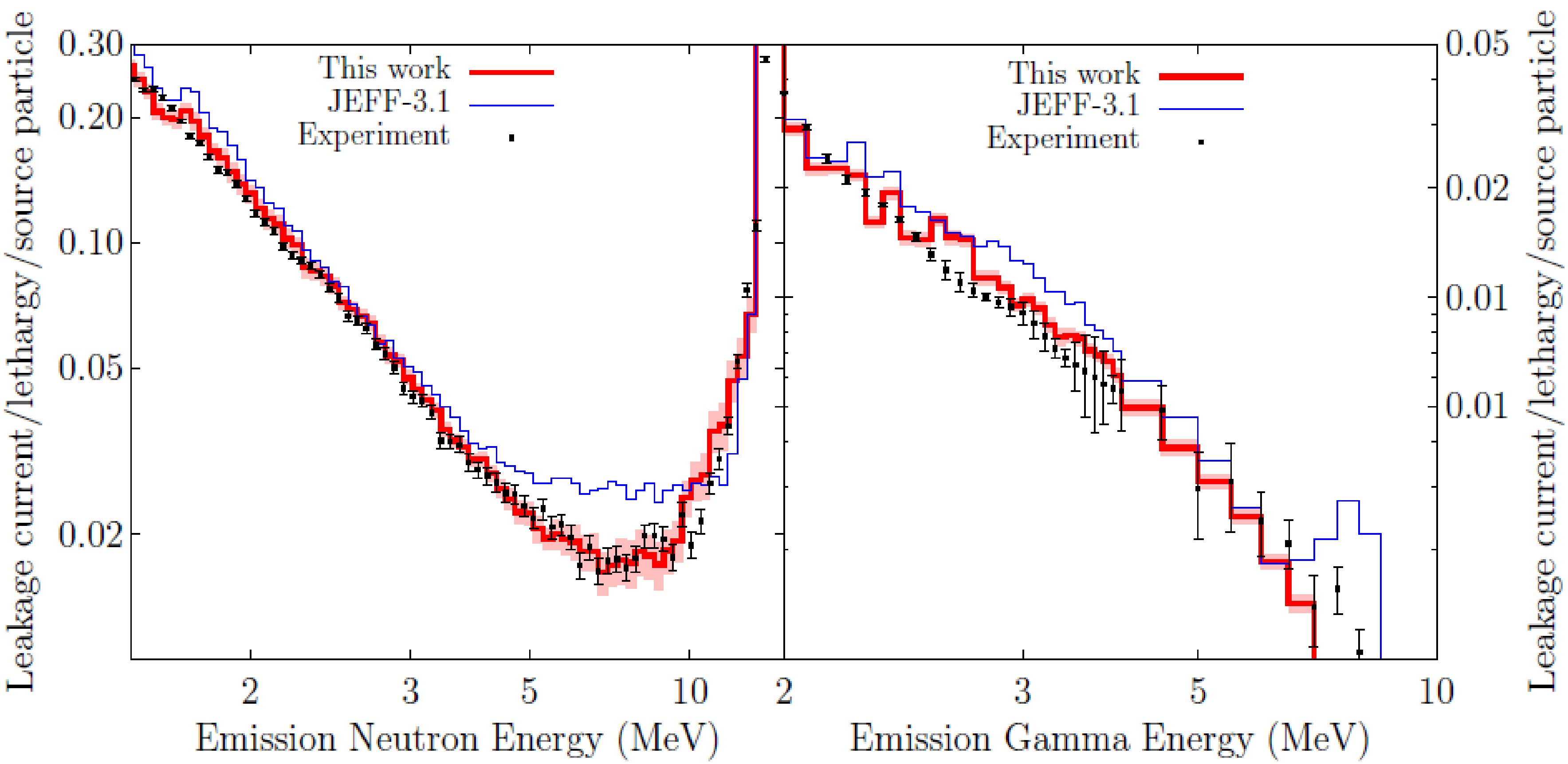
SFR void coefficient

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



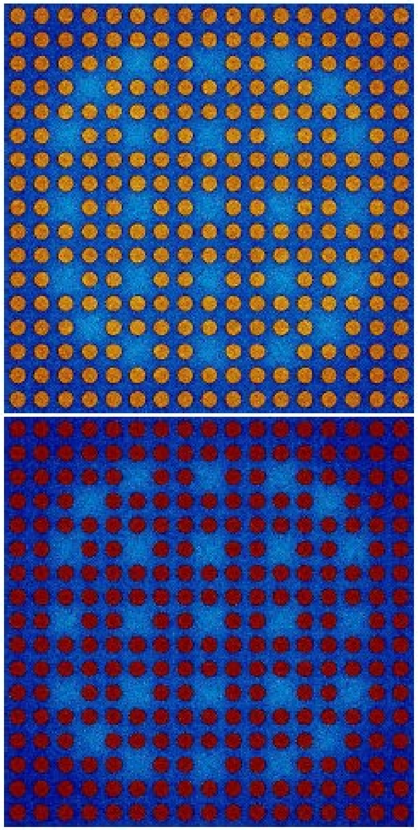
TMC for fusion: Optimized Cu63,65 file vs Oktavian: integral performance

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).



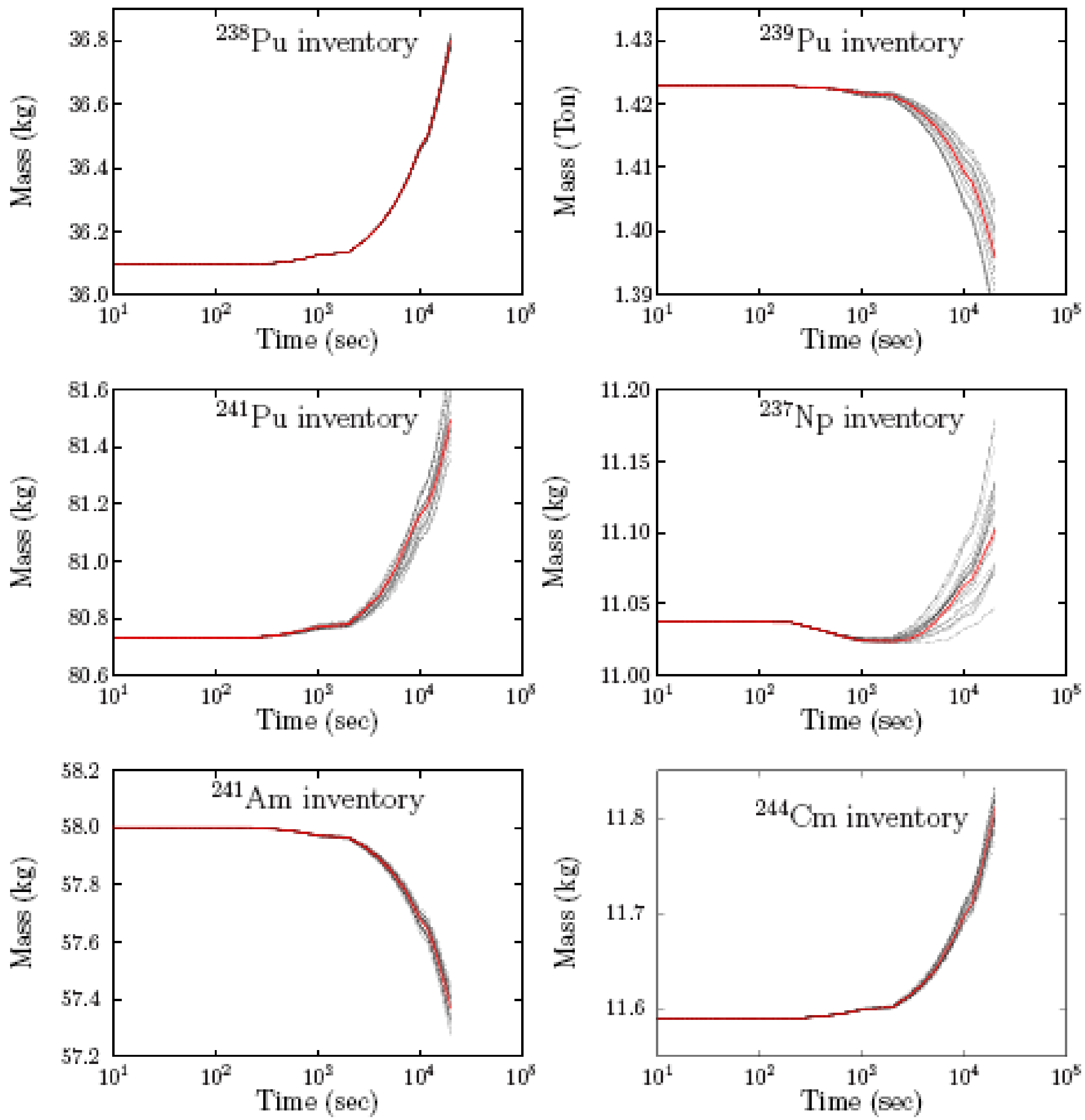
PWR fuel assembly model

Based on a Westinghouse 3-loop PWR-design, 4.8 % enrichment in ^{235}U, rods of zirconium alloy, 17x17, 4 m in length and 21.5 cm in width, fuel temperature of 930 Kelvin, cladding and moderator at 590 Kelvin, constant boric acid concentration of 500 ppm.



Coolant in blue, depletion in the lattice is indicated by a darker color or rods

Calculate uncertainties in inventory with Serpent



PWR burn-up calculations

D. Rochman, A.J. Koning and D. da Cruz, ``Propagation of 235,236,238U and 239Pu nuclear data uncertainties for a typical PWR fuel element'', Nuclear Technology 179, no. 3, 323-338 (2012).

Publications

Get'm all at ftp://ftp.nrg.eu/pub/www/talys/bib_koning/publications.html

Examples:

- D.F. da Cruz, D. Rochman, and A.J. Koning, ``Uncertainty analysis on reactivity and discharged inventory due to U235,238, Pu239,240,241 and fission products nuclear data uncertainties - application to a pressurized water reactor fuel assembly'', to be published (2013).
- D. Rochman, A.J. Koning, J. Kopecky, J.-C. Sublet, P. Ribon and M. Moxon, ``From average parameters to statistical resolved resonances'', Ann. Nuc. En. 51, 60 (2013).
- A.J. Koning and D. Rochman, ``Modern nuclear data evaluation with the TALYS code system'', Nucl. Data Sheets 113, 2841 (2012).
- D. Rochman and A.J. Koning, ``Random adjustment of the H in H2O neutron thermal scattering data'', Nucl. Sci. Eng. 172, no. 3, 287-299 (2012).
- D. Rochman, A.J. Koning and D. da Cruz, ``Propagation of 235,236,238U and 239Pu nuclear data uncertainties for a typical PWR fuel element'', Nuclear Technology 179, no. 3, 323-338 (2012).
- A.J. Koning and D. Rochman, ``Modern nuclear data evaluation: Straight from nuclear physics to applications'', Journ. Kor. Phys. Soc. 59, no. 23, 773 (2011).
- D. Rochman and A.J. Koning, ``How to randomly evaluate nuclear data: a new method applied to Pu-239'', Nucl. Sci. Eng. 169(1), 68 (2011).
- D. Rochman, A.J. Koning, S.C. van der Marck, A. Hogenbirk and C.M. Sciolla, ``Nuclear data uncertainty propagation: Perturbation vs. Monte Carlo'', Ann. Nuc. En. 38, 942 (2011).
- D. Rochman, A.J. Koning, D.F. da Cruz, ``Uncertainties for the Kalimer Sodium Fast Reactor: void coefficient, keff, Beff, burn-up and radiotoxicity'', Jap. Journ. Sci. Techn. 48 (8) 1193 (2011).

Conclusions

- By simultaneously developing and maintaining:
  1. A complete modern nuclear data library: TENDL
  2. An unprecedented integral validation scheme with integral experiments and benchmarks
  3. A Total Monte Carlo method applied on well-established Monte Carlo and deterministic reactor codes
  4. An extension to full core analyses

complete probability distributions (uncertainties, covariances) for many reactor and inventory quantities of interest can be obtained.

- Total Monte Carlo: If we can calculate it once we can also calculate it 1000 times, randomly varying the input.
- Safety, uncertainty, risk and money are equivalent, also in the nuclear world. Therefore, exact uncertainty propagation will be beneficial.