# Exact uncertainty propagation of nuclear data with Monte Carlo: Application to a PBMR

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*NRG, Petten, The Netherlands*

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## Contents

## Introduction: Motivations for a change

Usual procedures in uncertainty propagation imply:

- ☞ rigid format, fixed libraries of cross sections, simplification of covariances,
- ☞ need for processing, sensitivity and perturbation codes, group scheme,
- ☞ necessity of linearizing inherently nonlinear relationships, and so on…

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> *"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

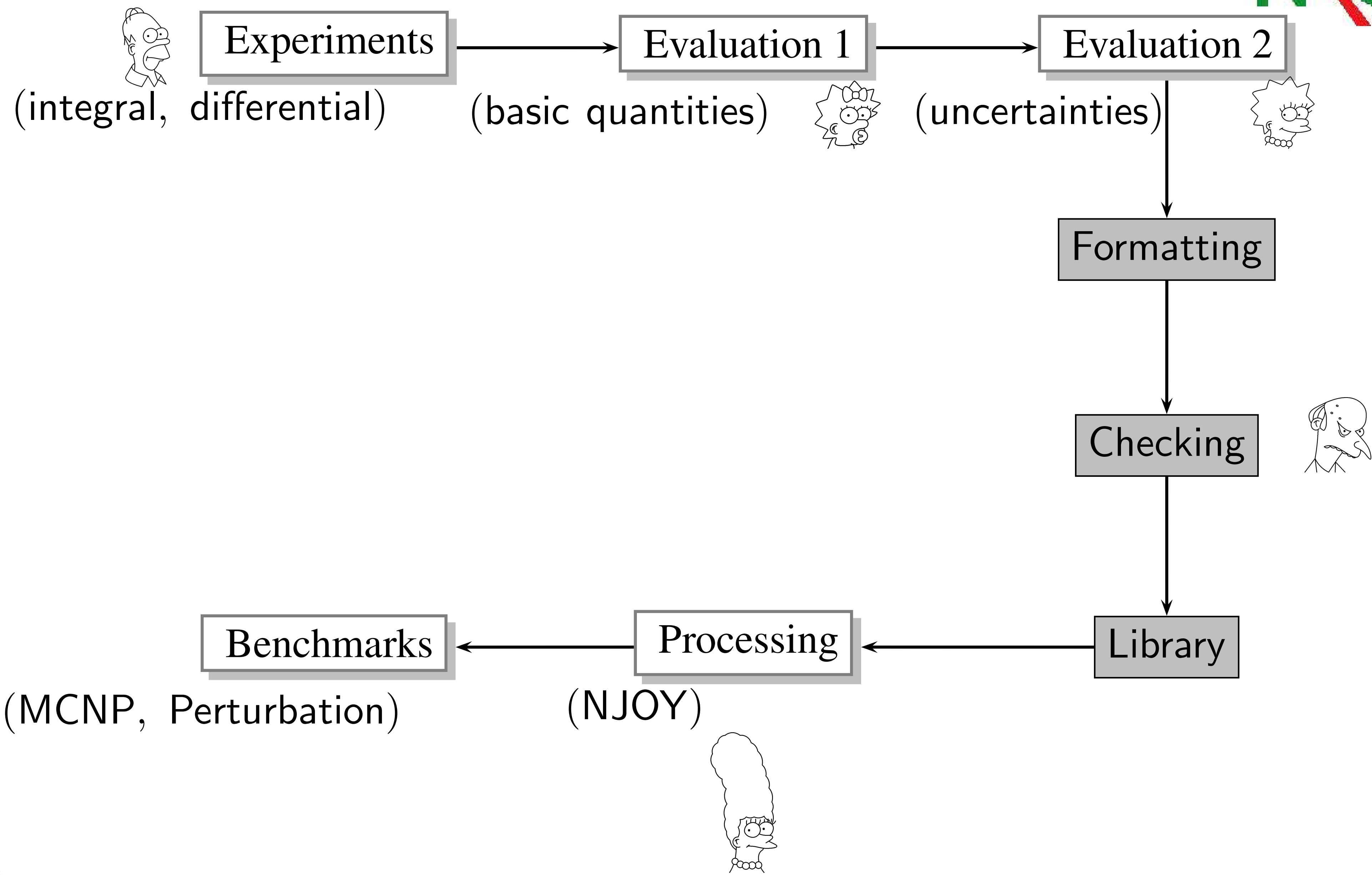
$\Longrightarrow$ Most straightforward way: Global Monte Carlo Approach !

# Total Monte Carlo Approach

- Stable Nuclear reaction code:**TALYS**
- Talys input parameters + uncertainties
- Resonance parameters + uncertainties

**Produce 5000 random,**
**complete ENDF-6 files per isotope**

# We are proposing a conceptual revolution



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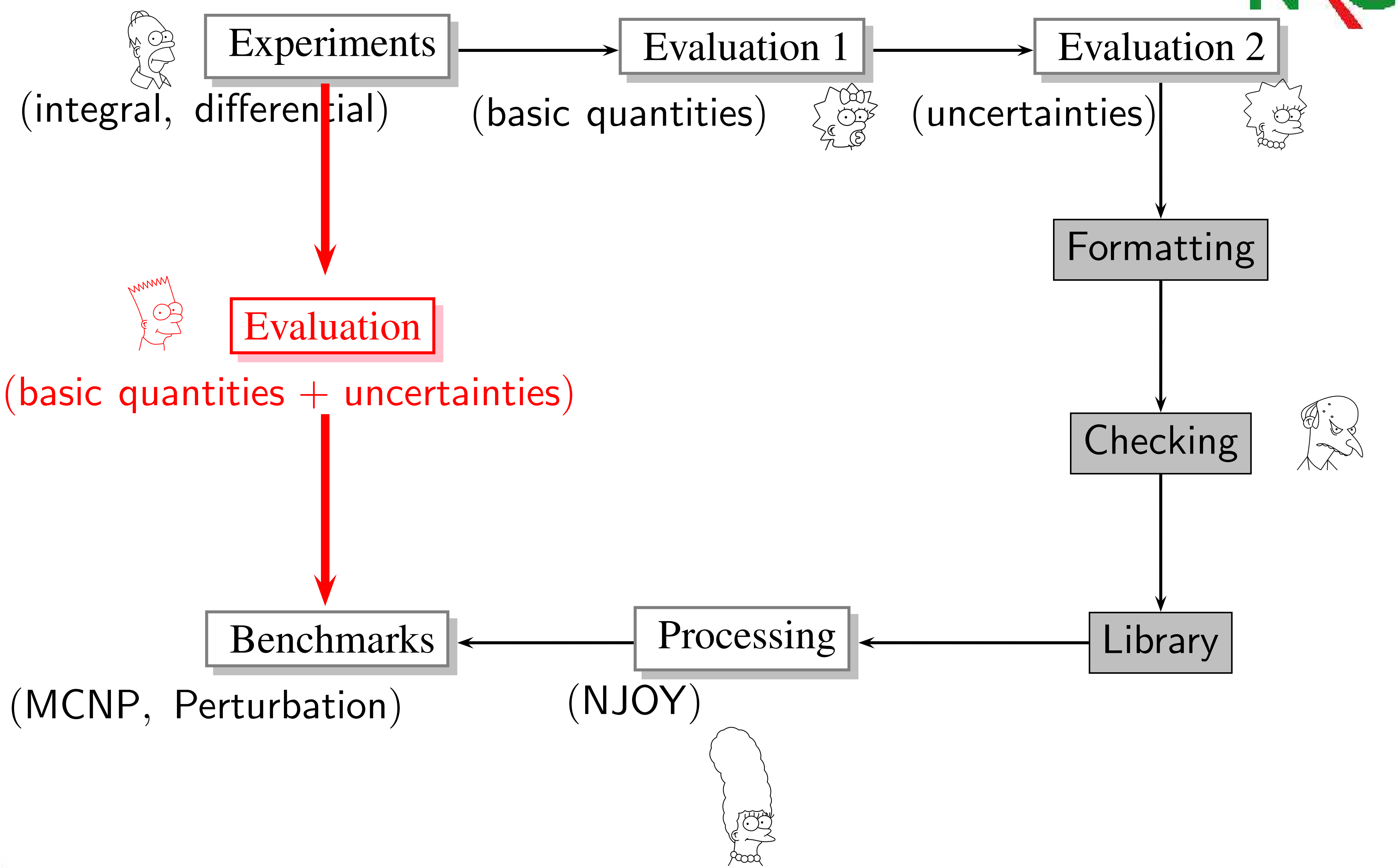

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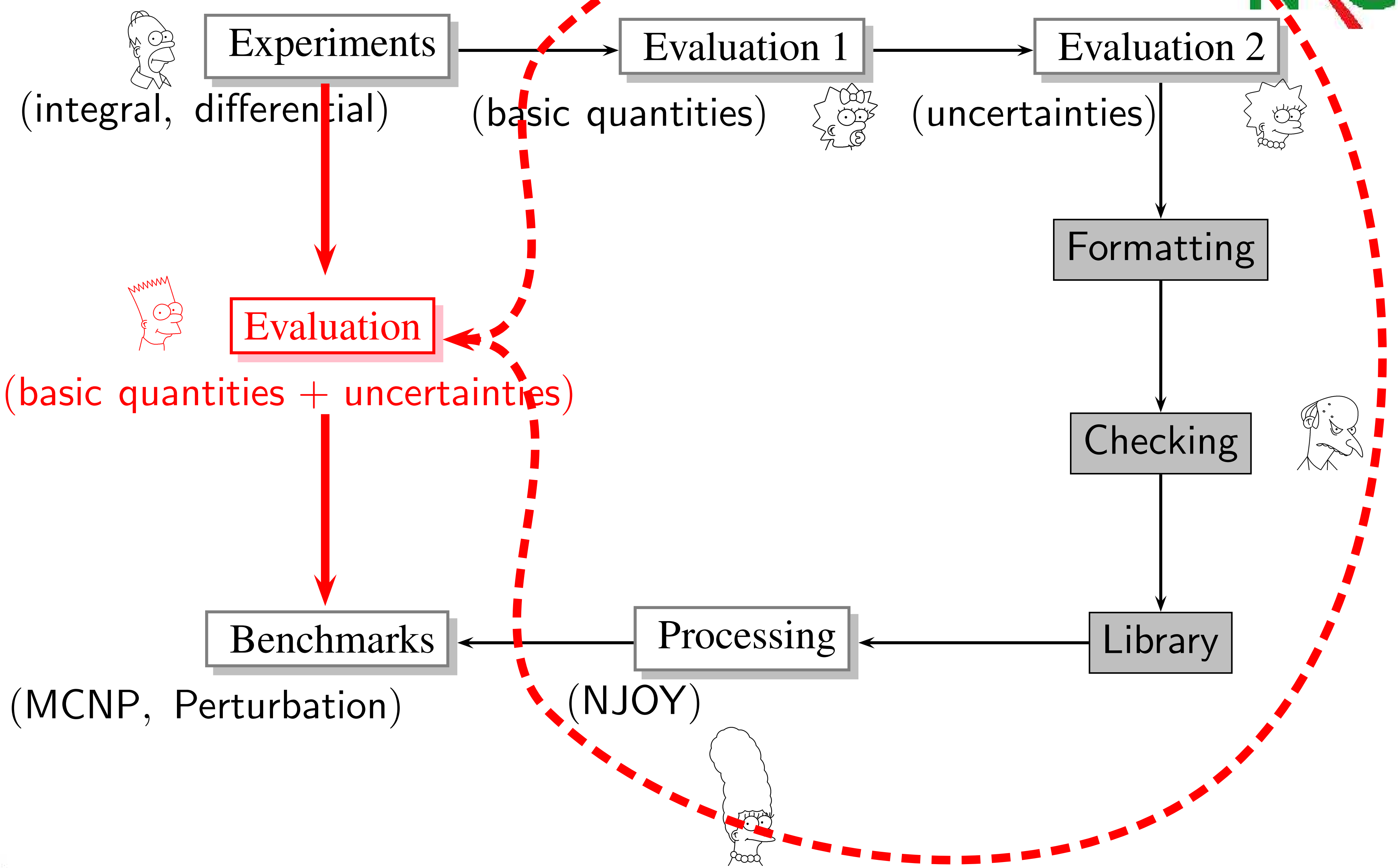
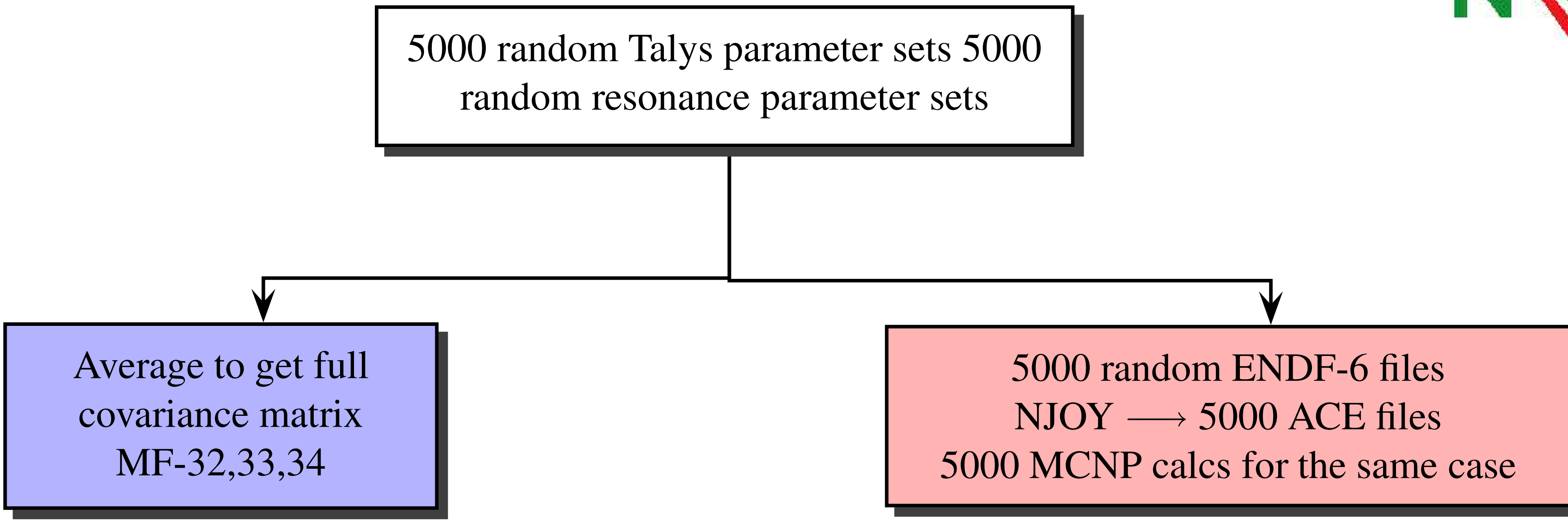


# New (and most simple) path




We have both routes, but one is easier and more exact to take than the second one.

## New (and most simple) path

5000 random Talys parameter sets 5000 random resonance parameter sets

Average to get full covariance matrix MF-32,33,34

5000 random ENDF-6 files
NJOY $\longrightarrow$ 5000 ACE files
5000 MCNP calcs for the same case

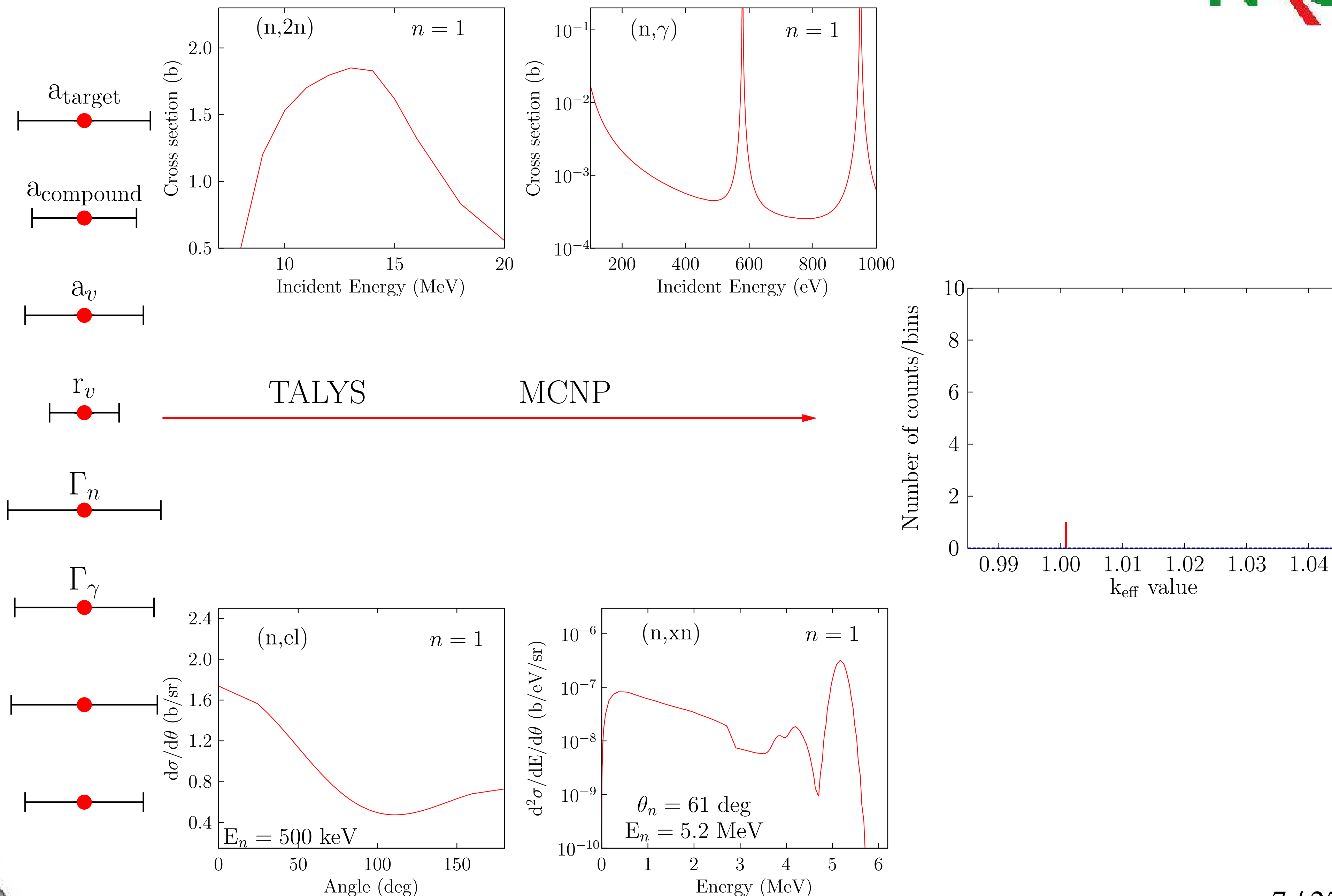
We have both routes, but one is easier and more exact to take than the second one.

Problem 1: ENDF format for covariances for fission yields, thermal scattering, branching ratios, DDX, $\gamma$-production

Problem 2: Processing of these covariances

Problem 3: Neutronics with covariances: perturbation codes. Are these generally available and working?

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



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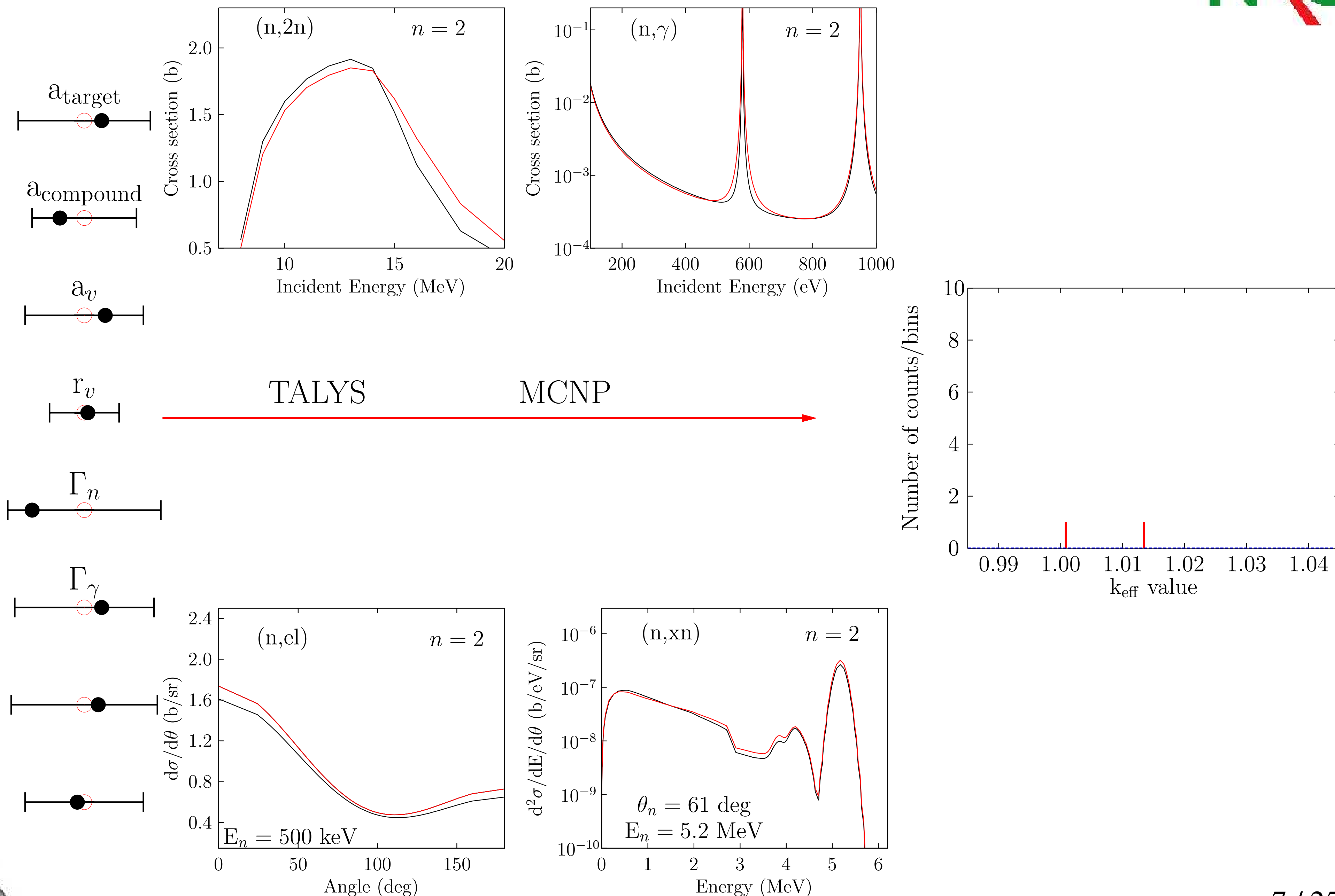

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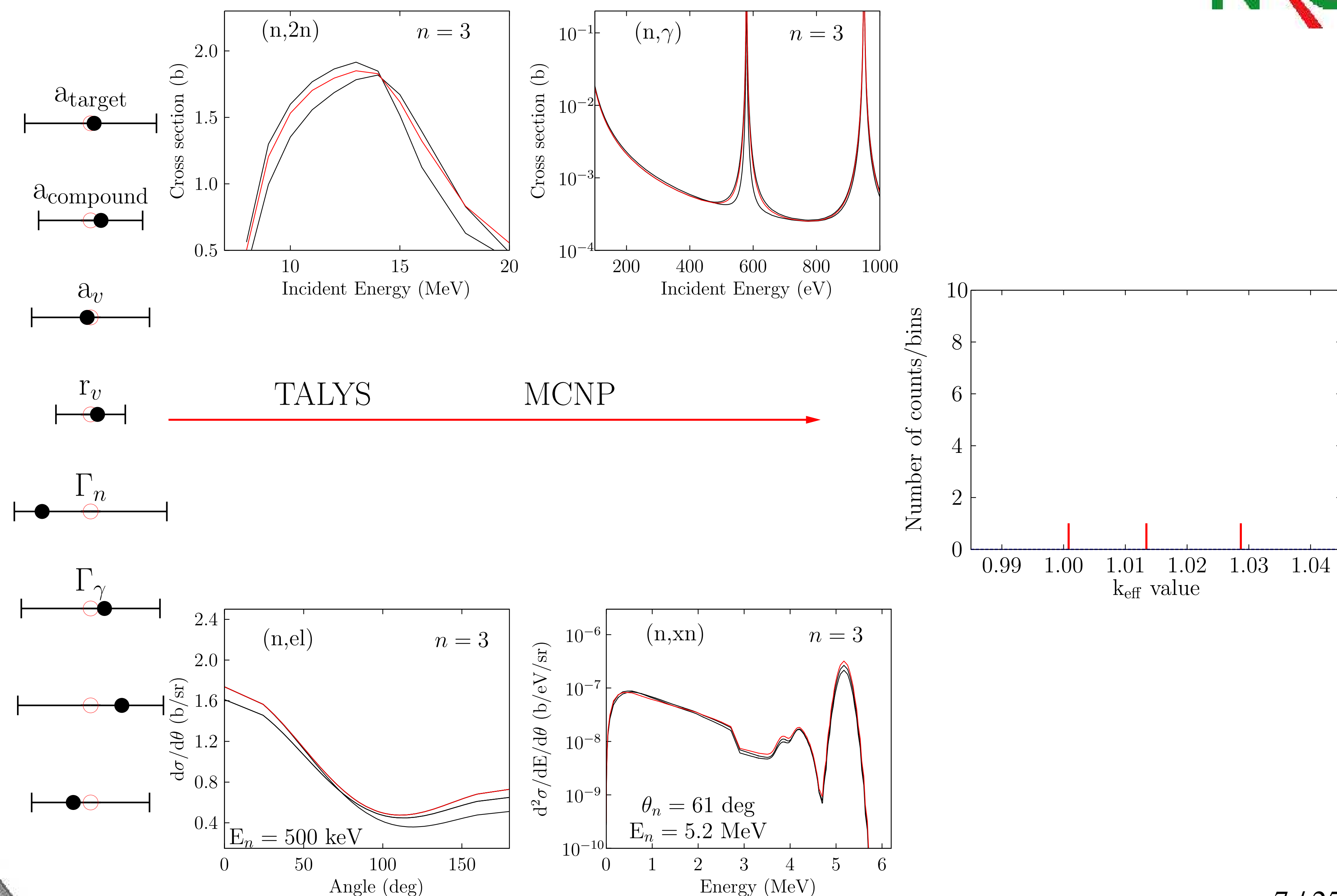

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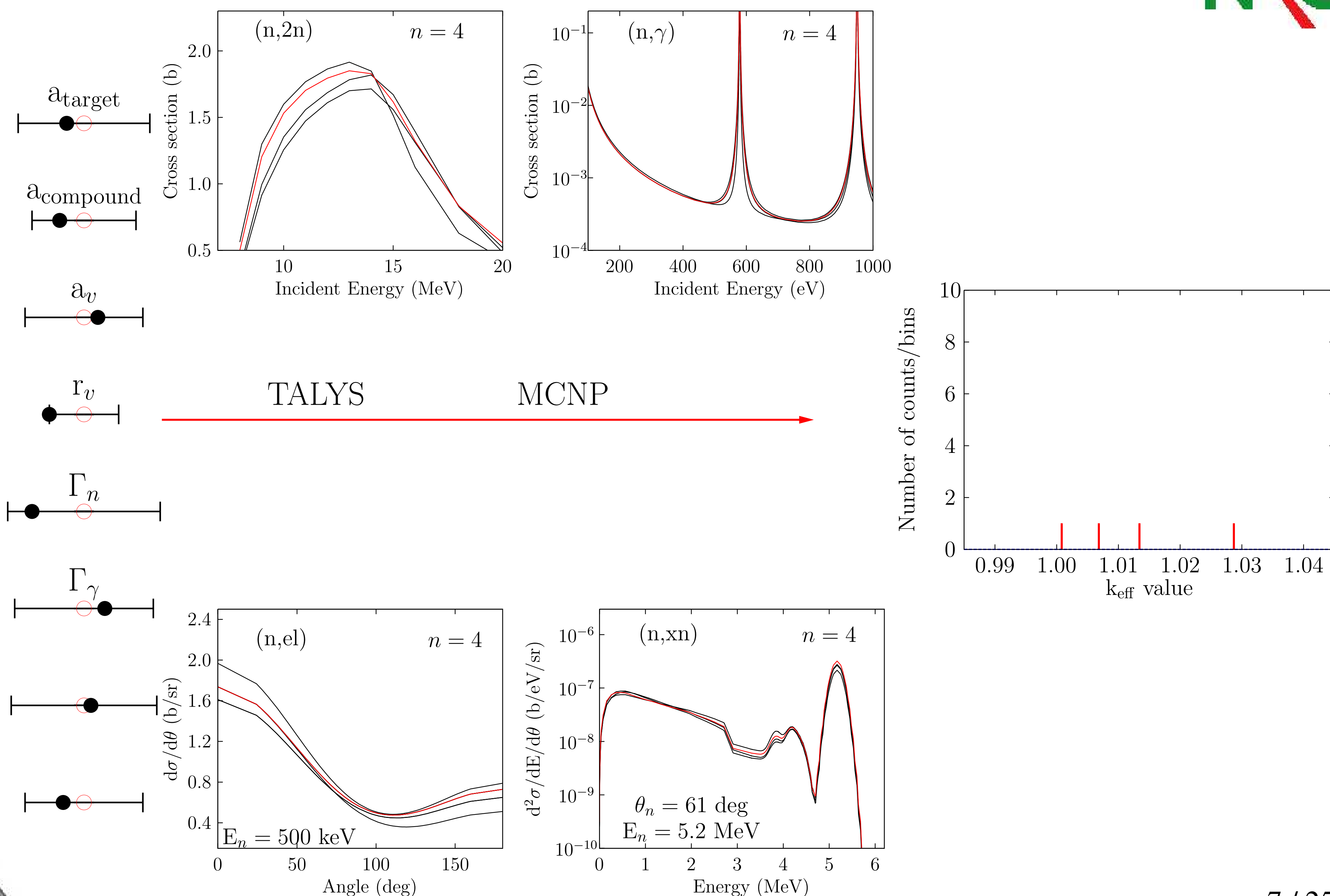

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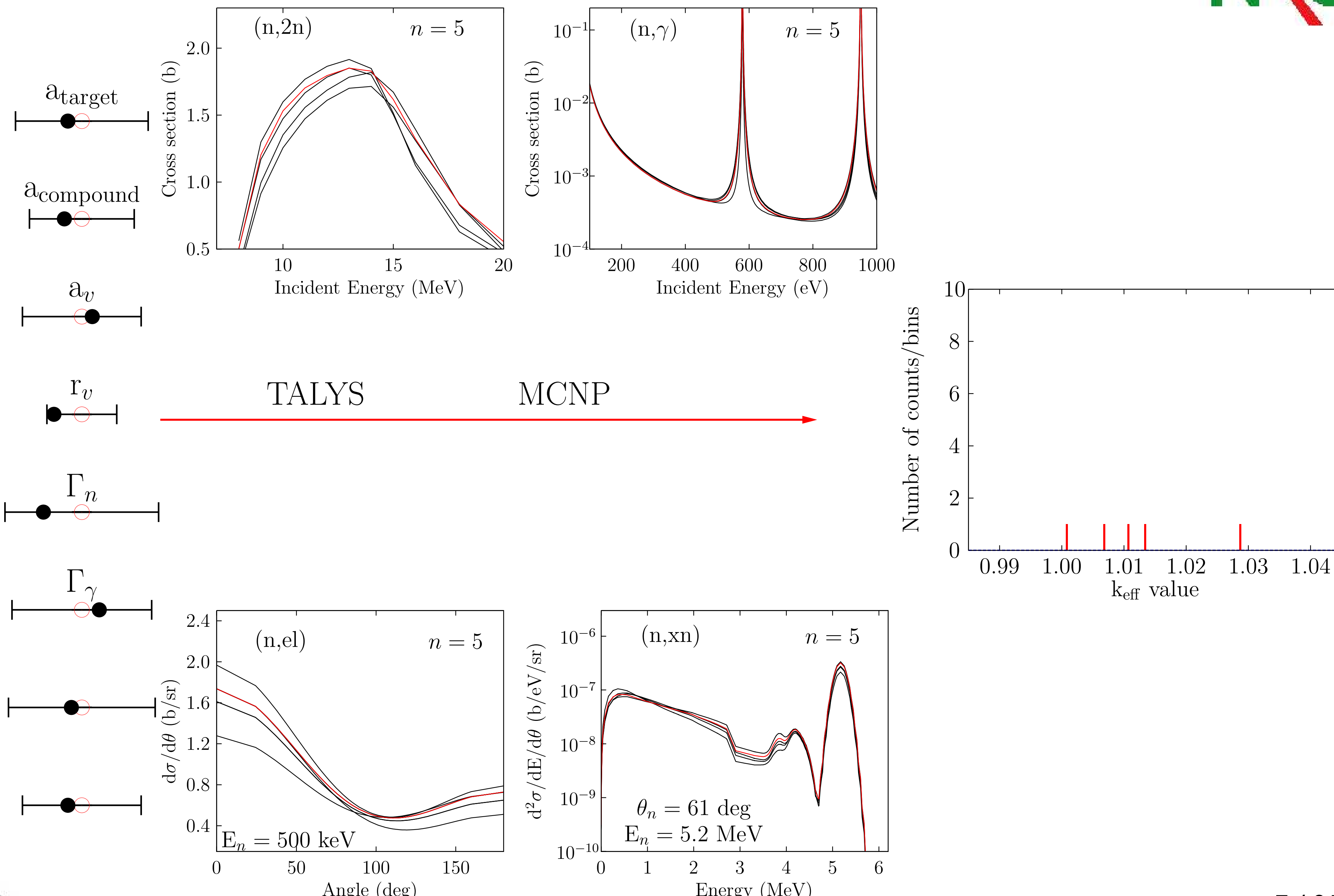

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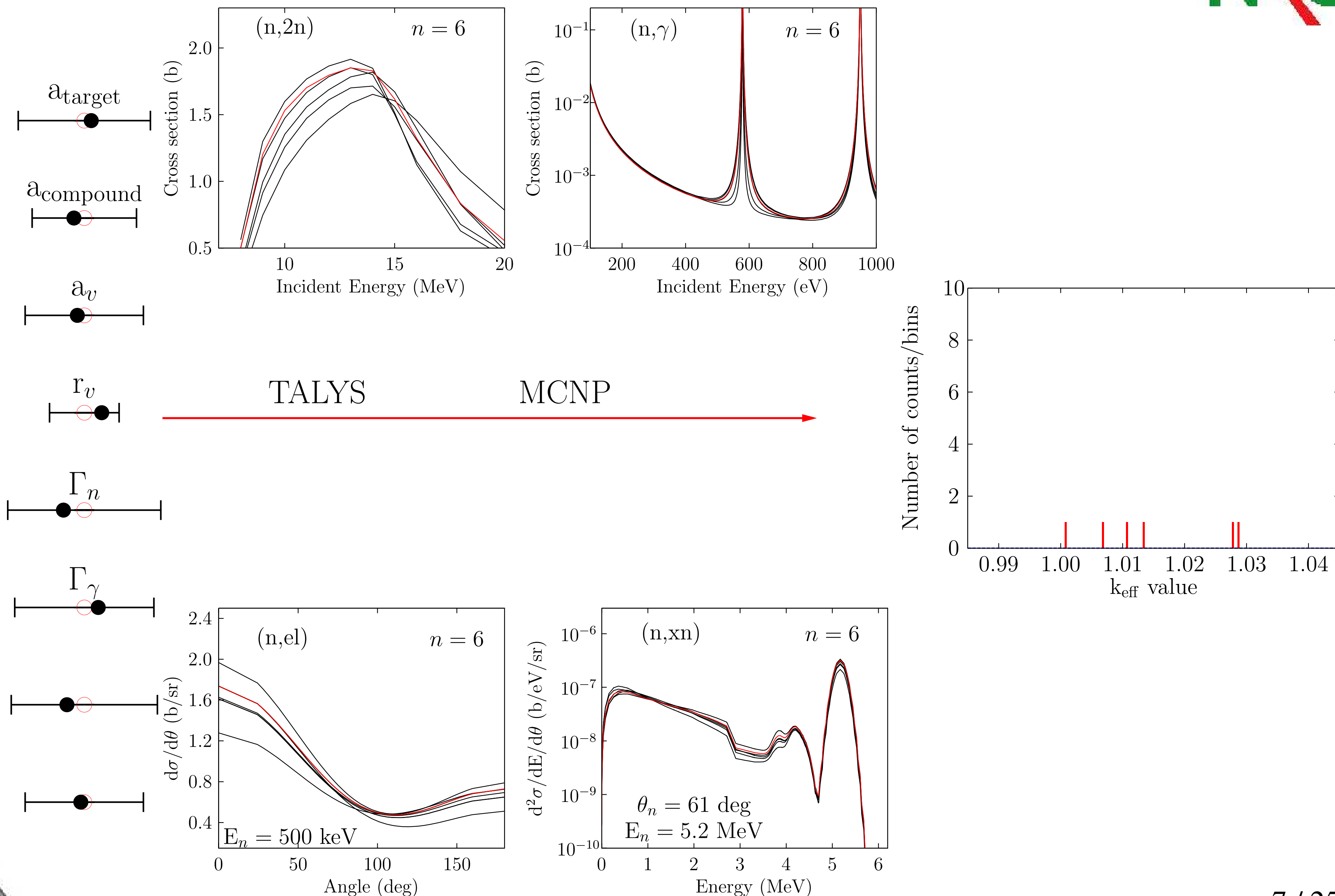

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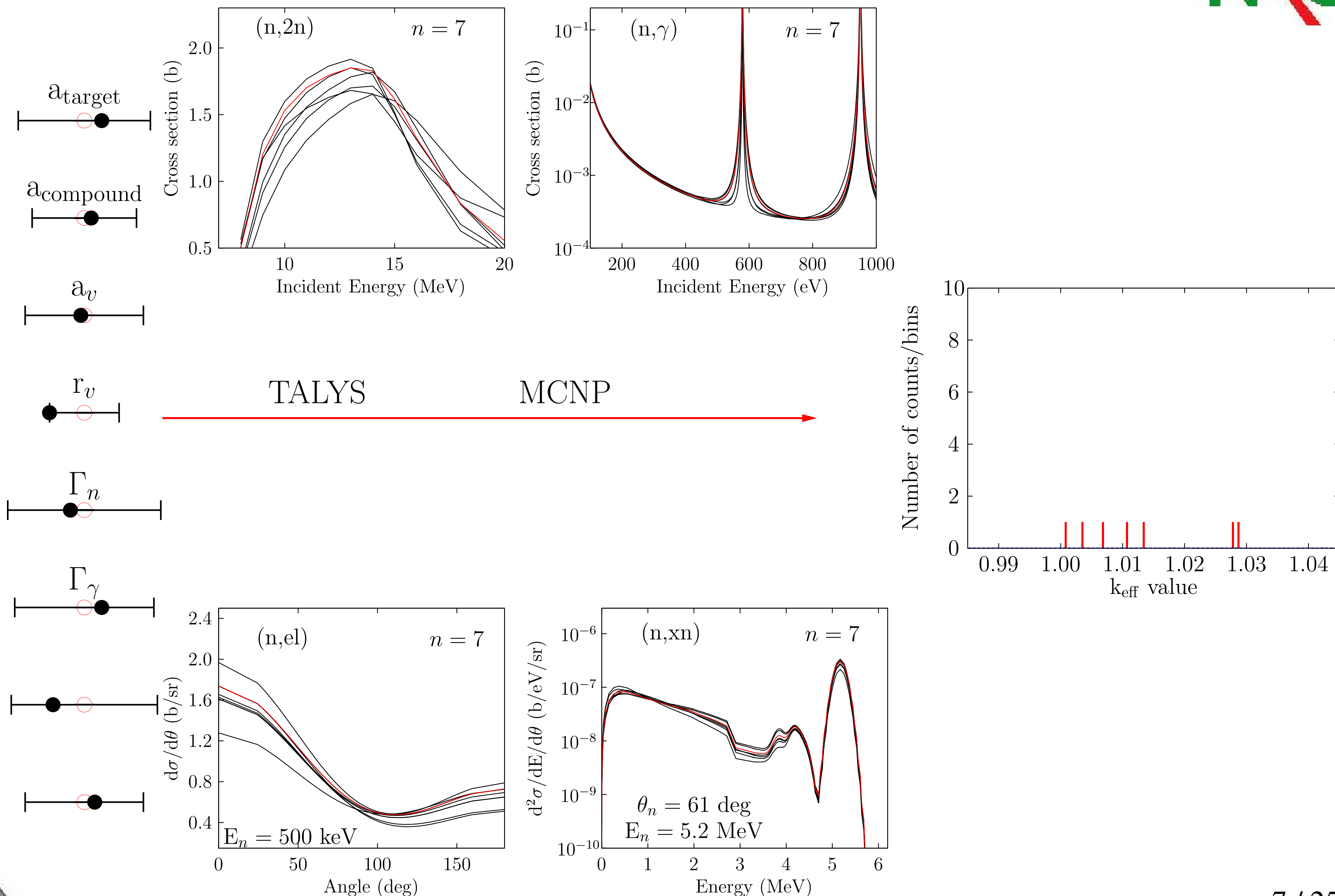

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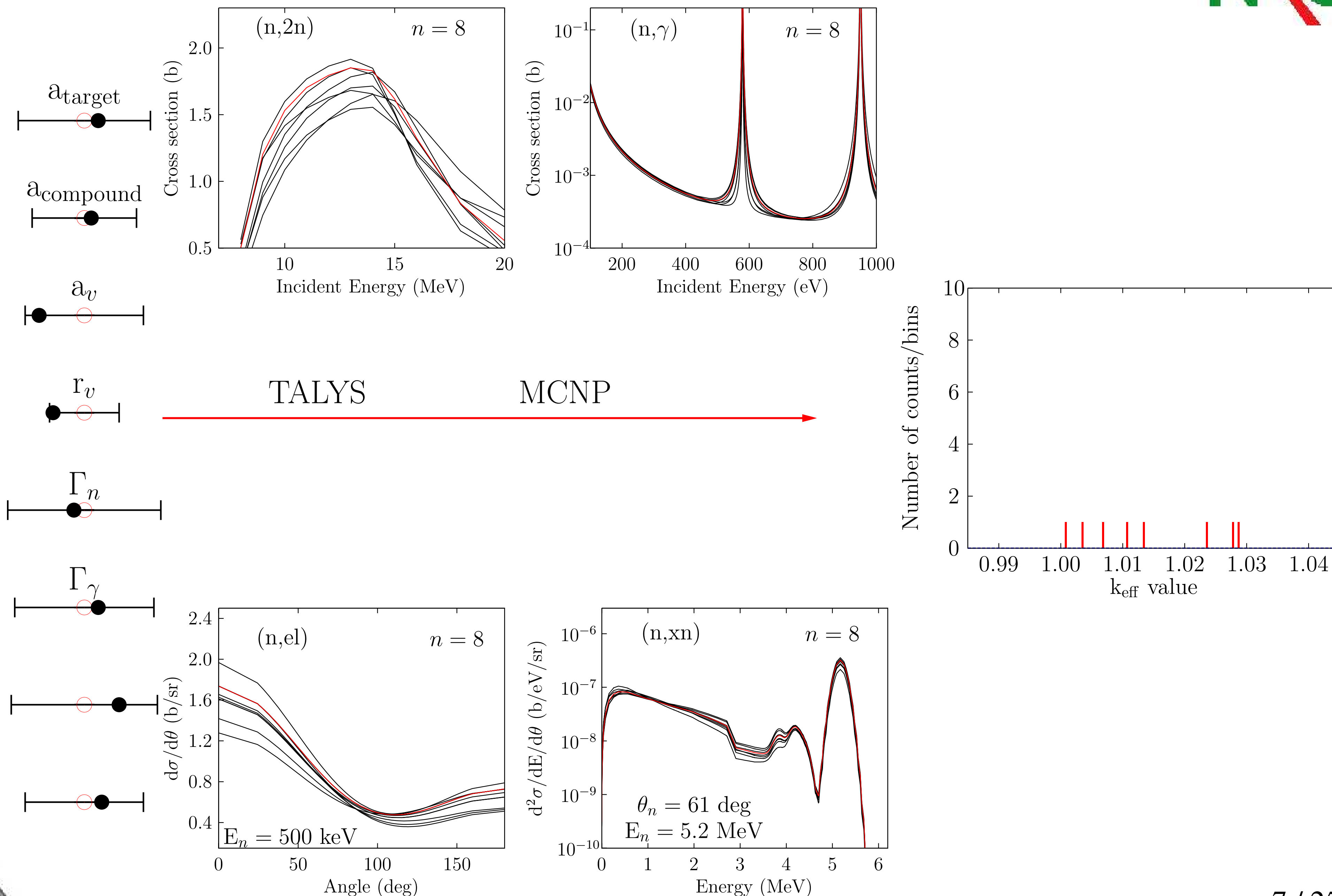

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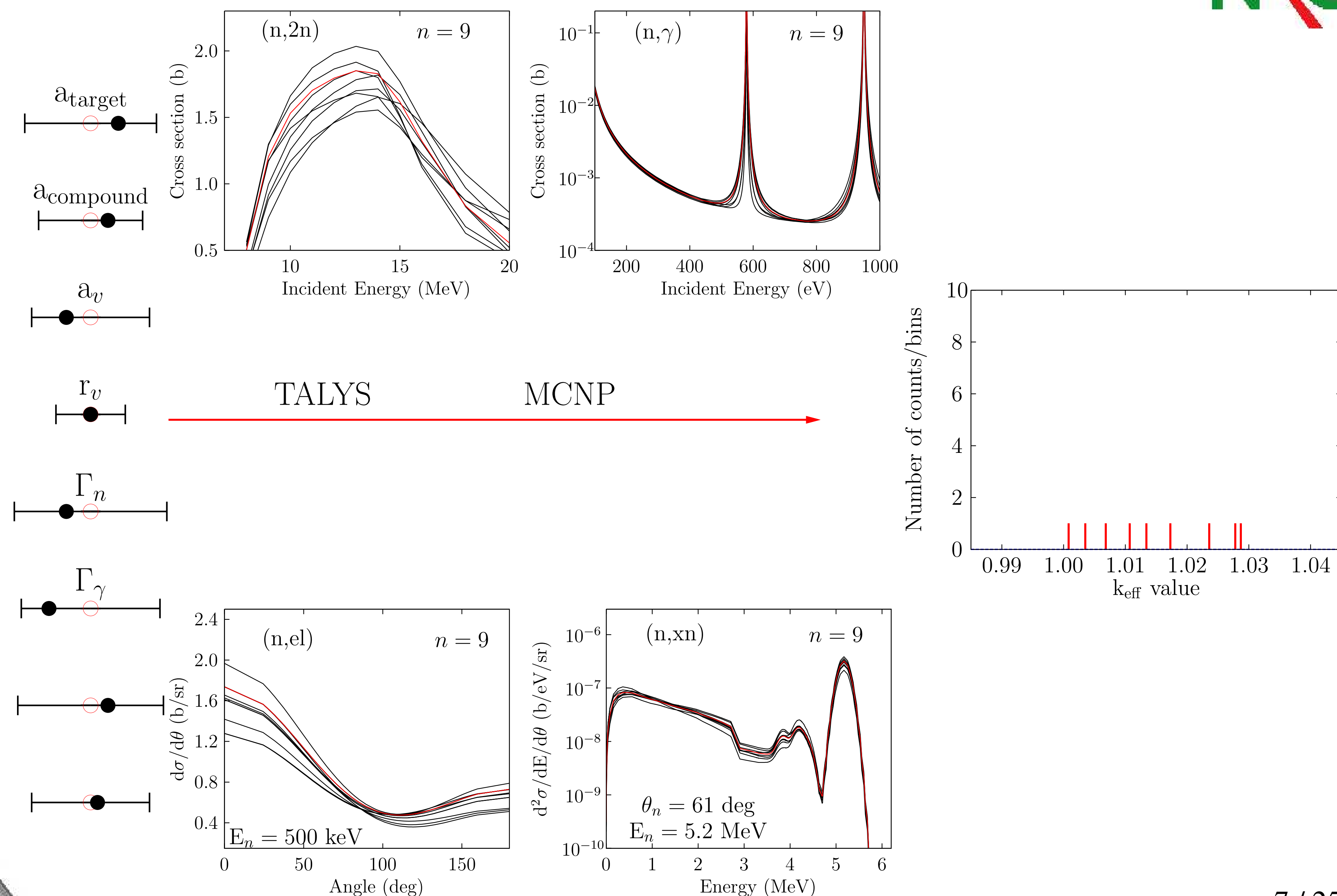

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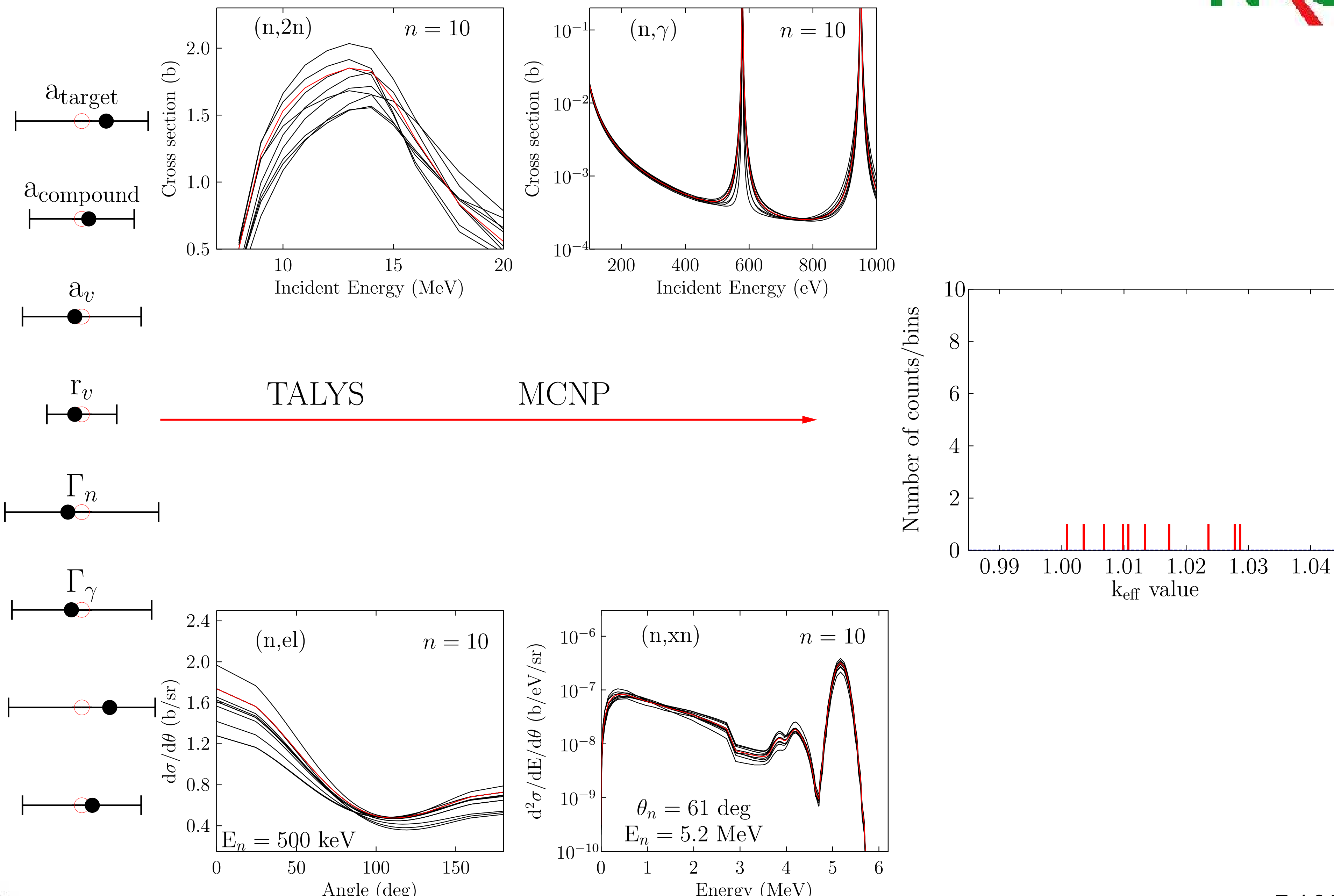

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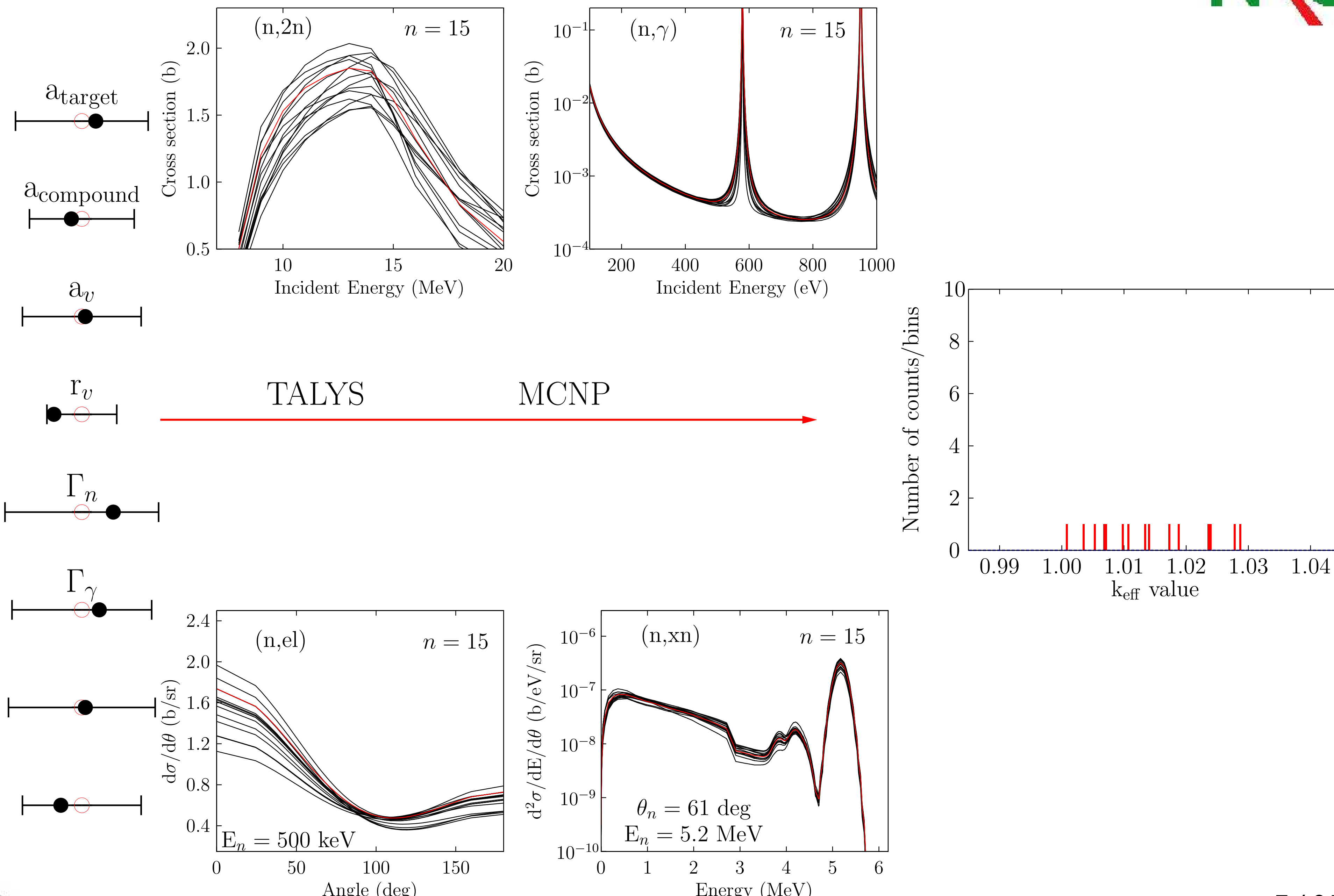

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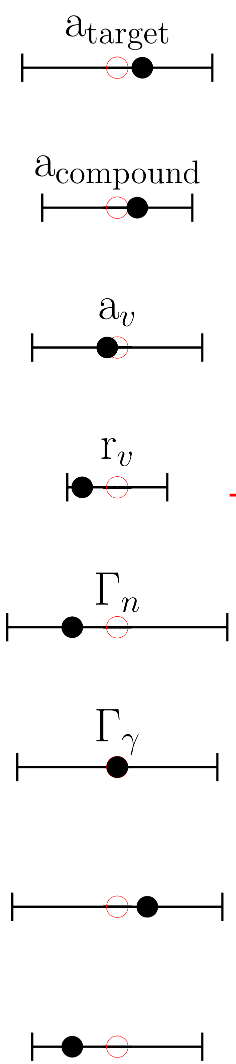
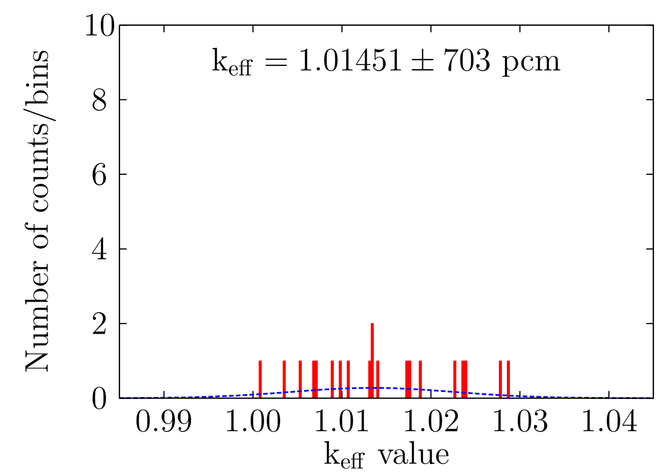



TALYS MCNP

$n = 20$



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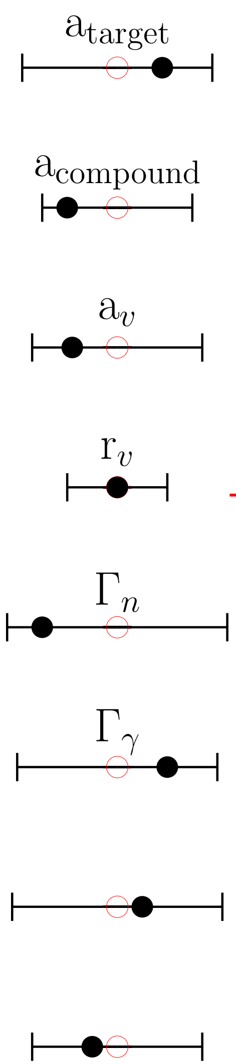
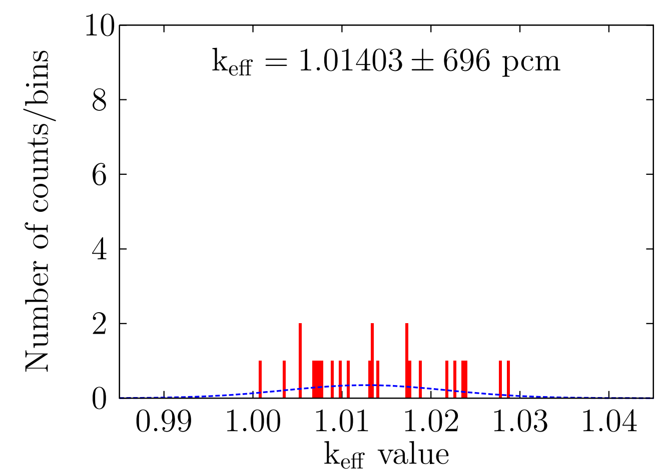



TALYS MCNP

$n = 25$



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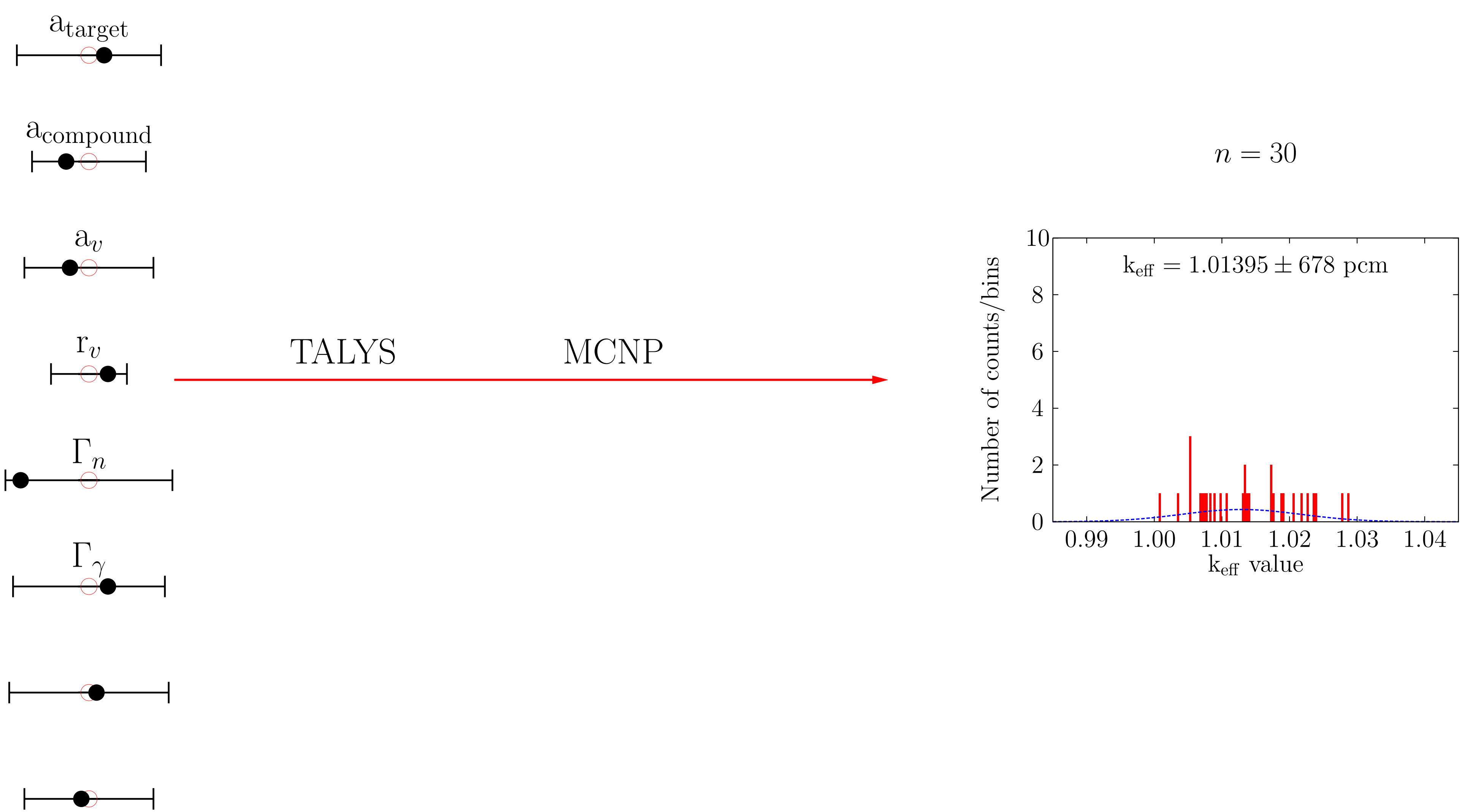

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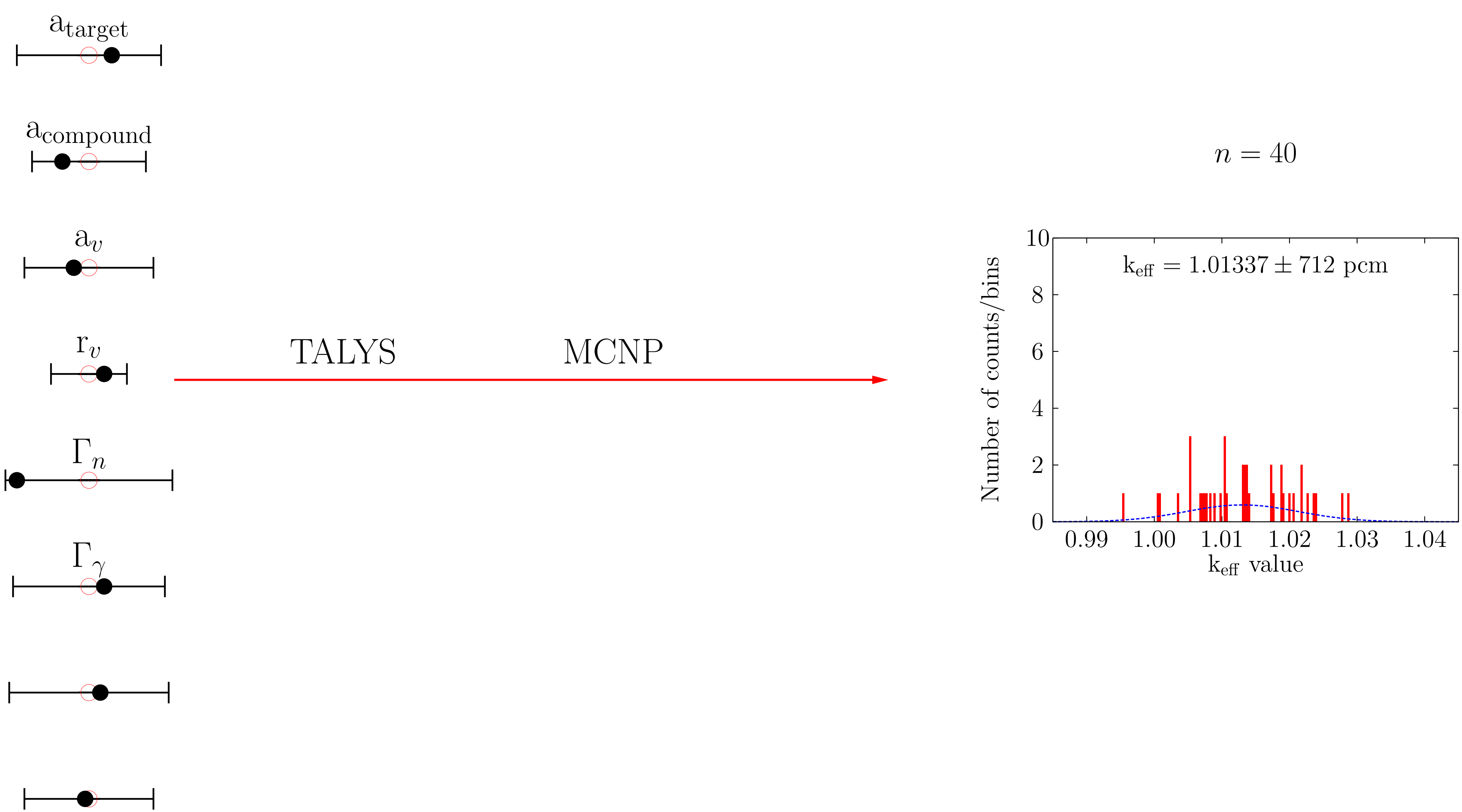

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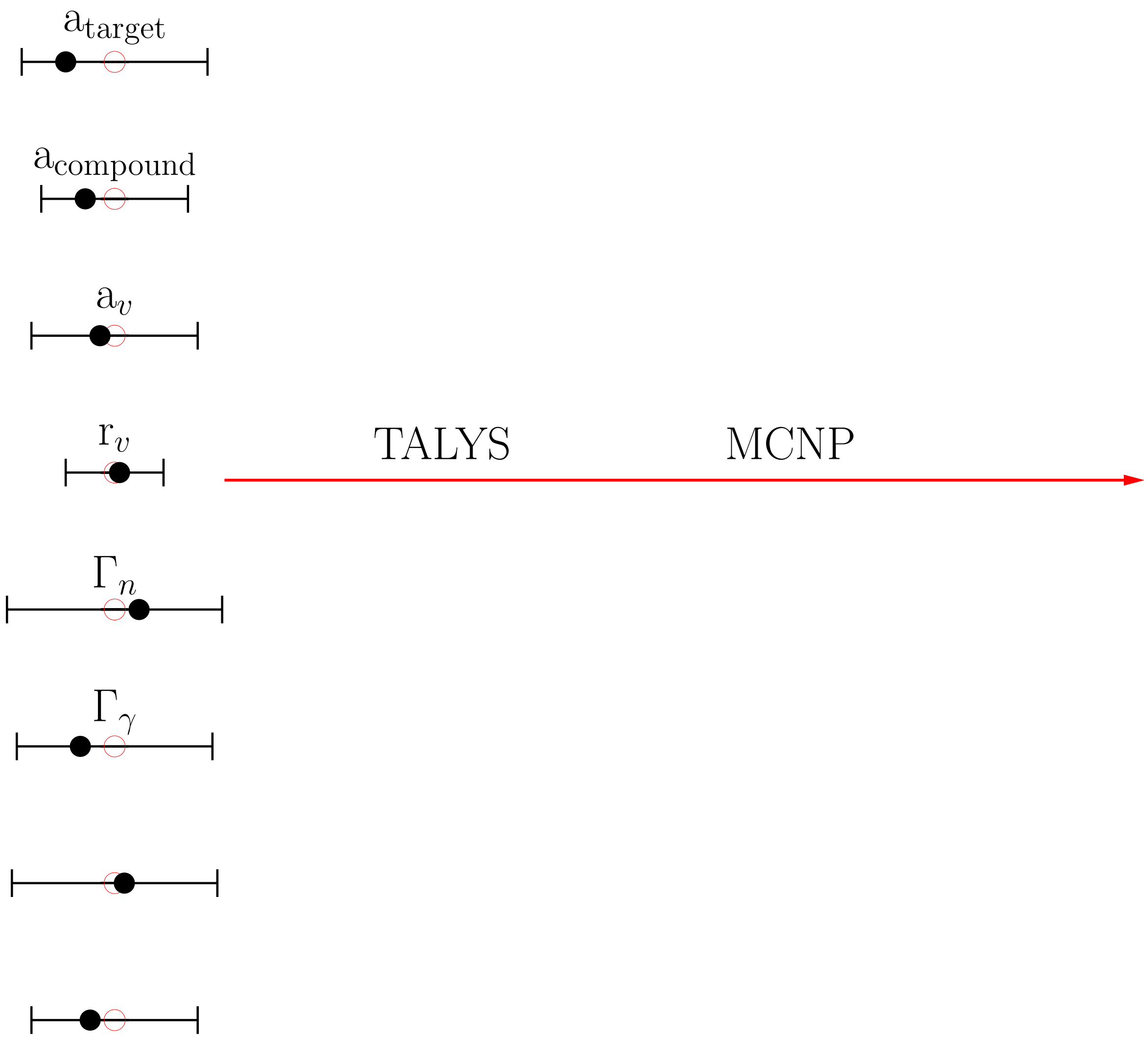
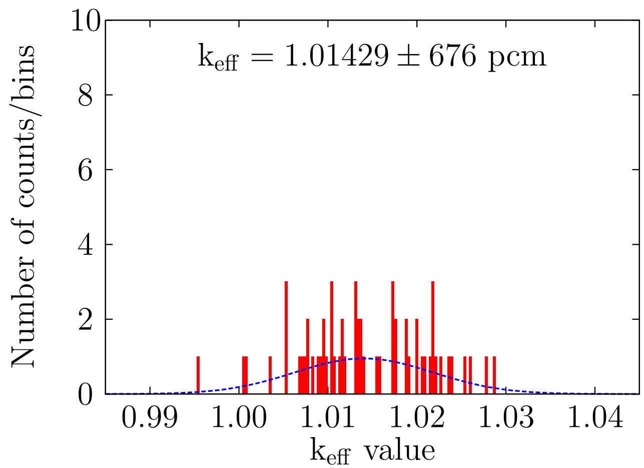



$n = 60$



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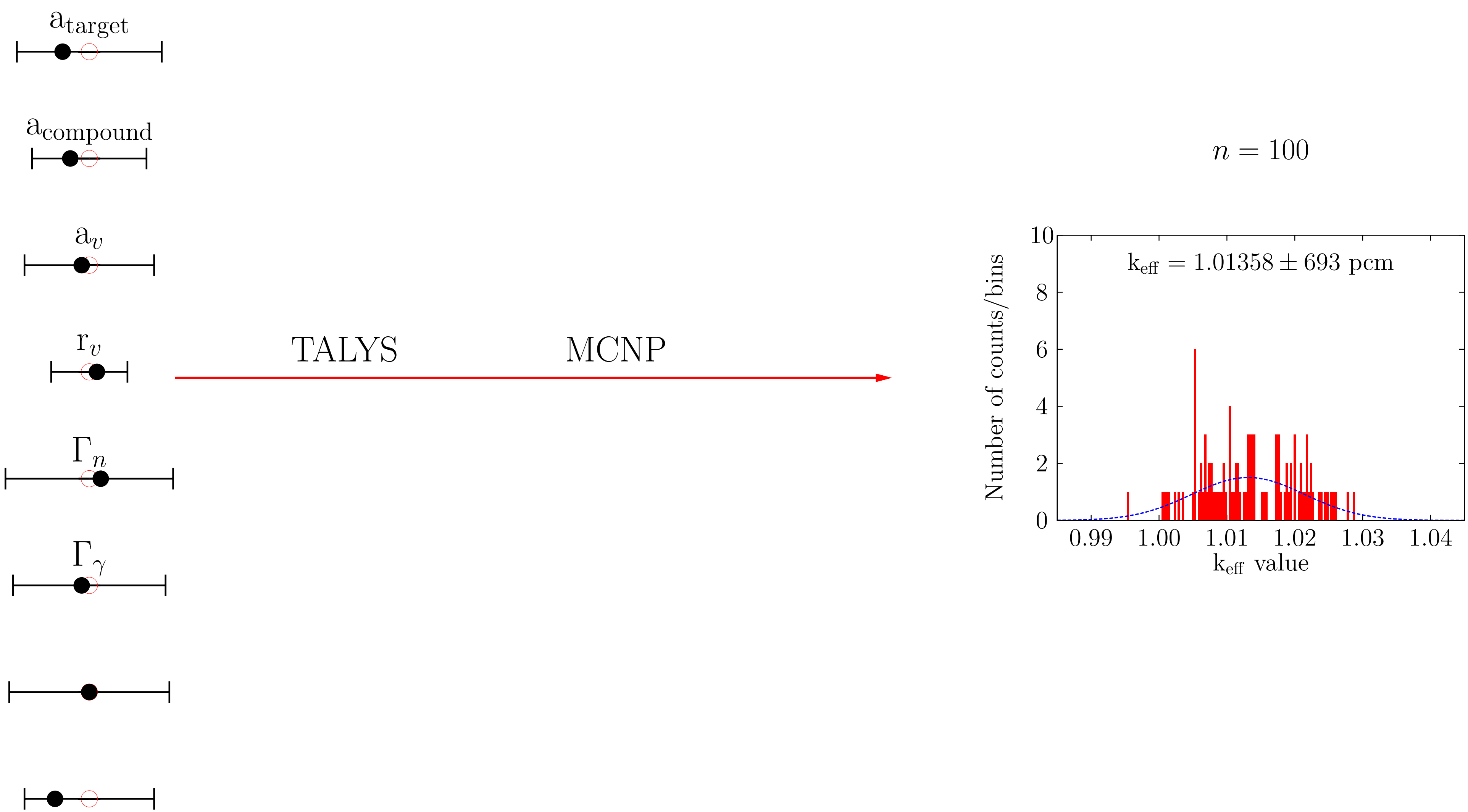

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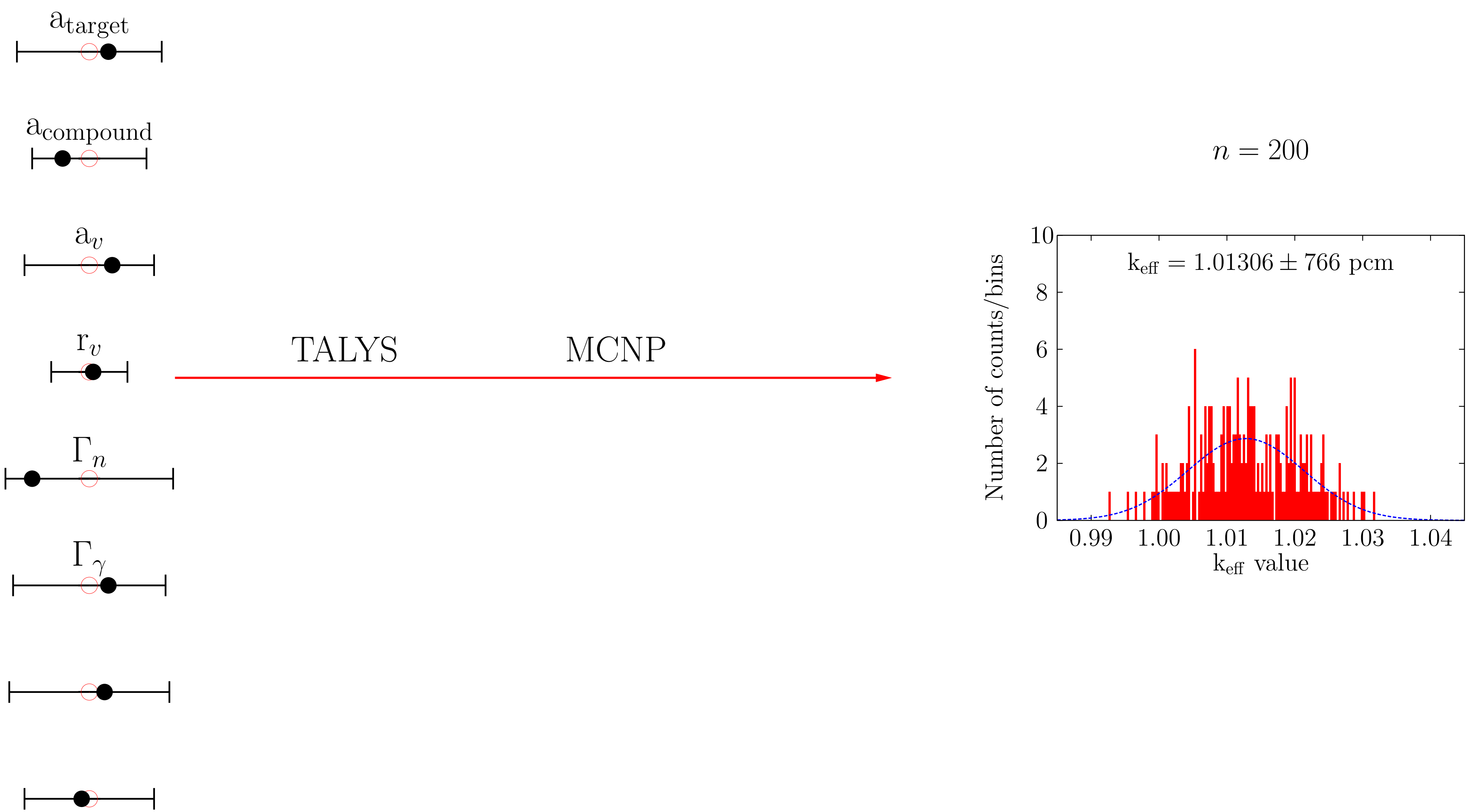

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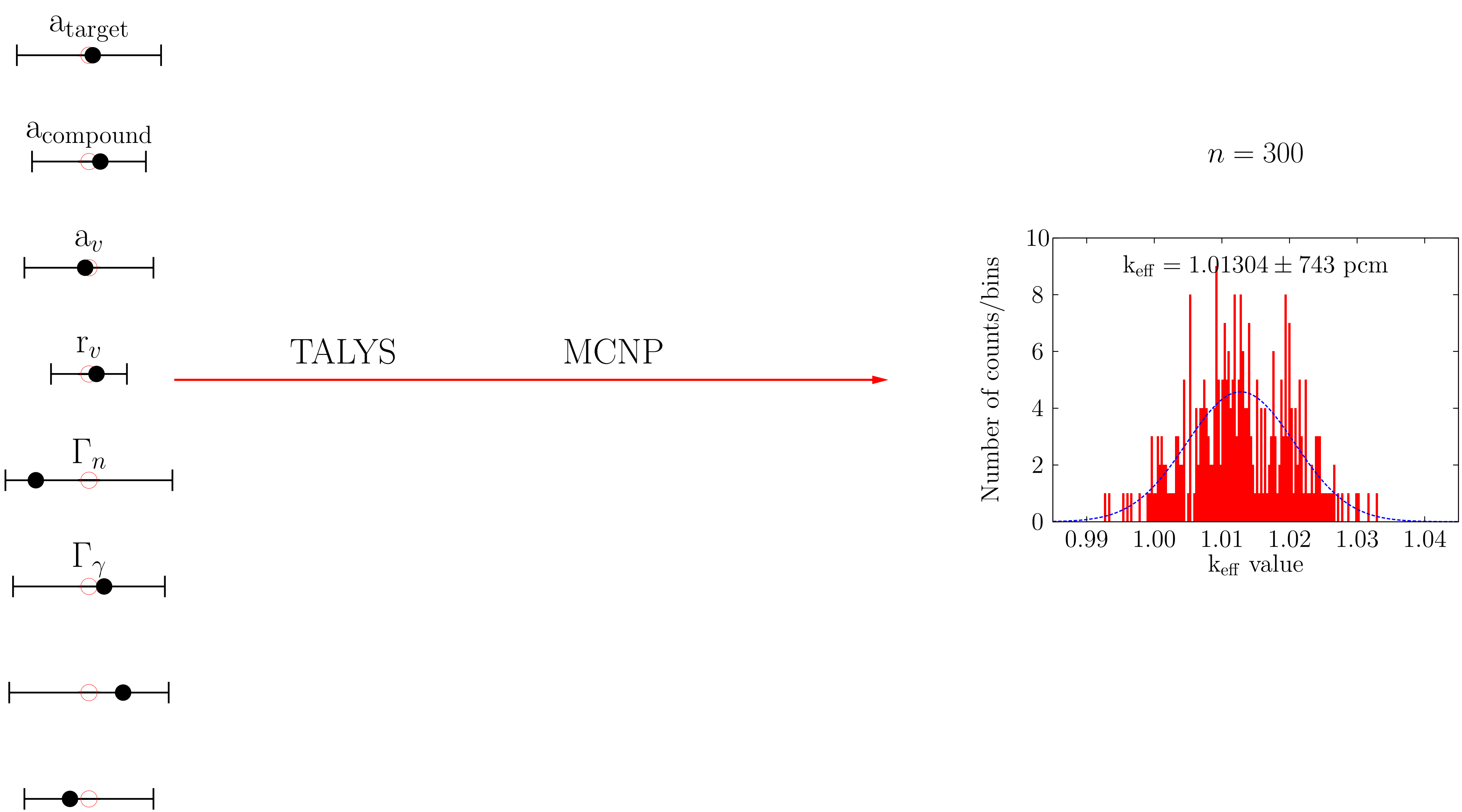

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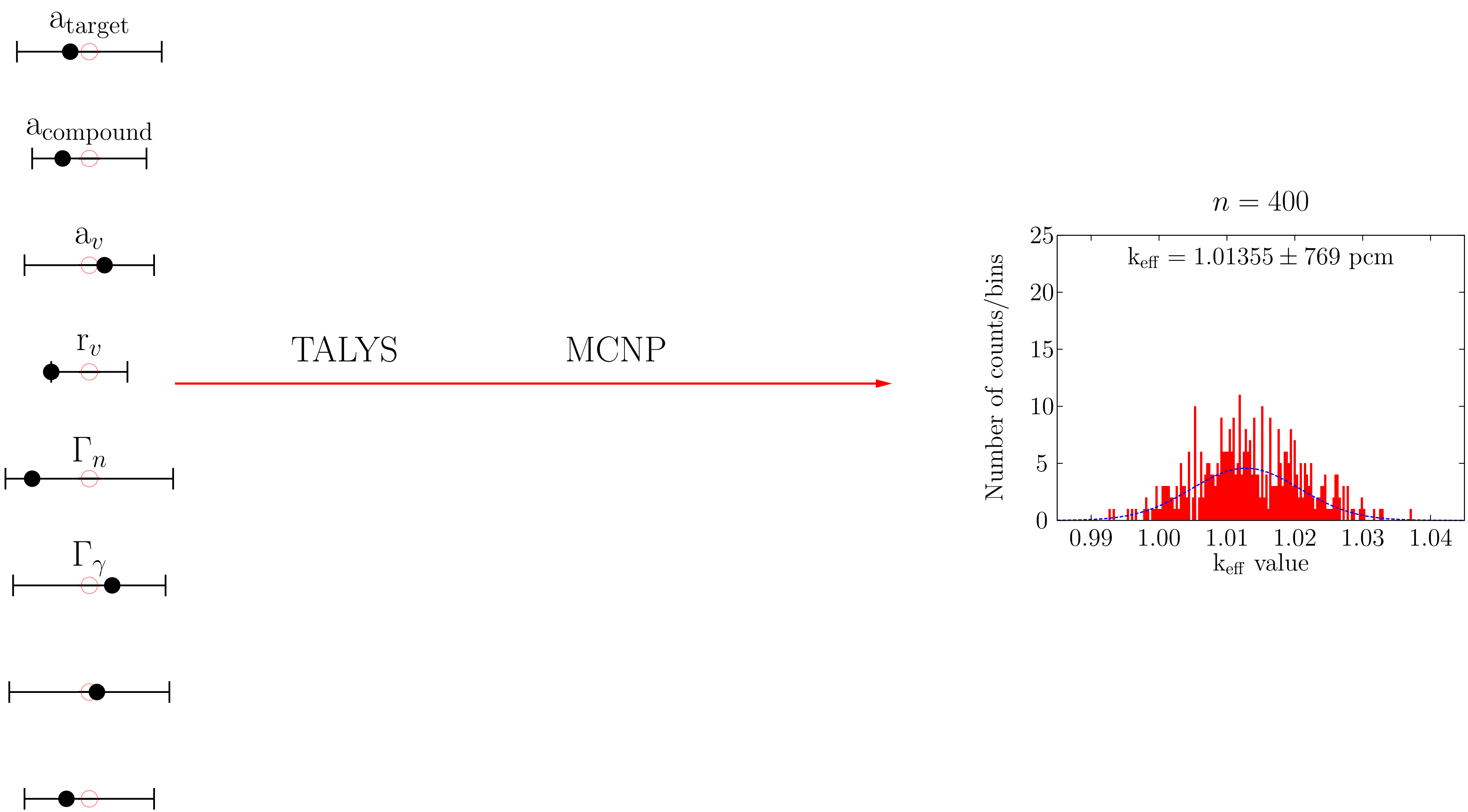

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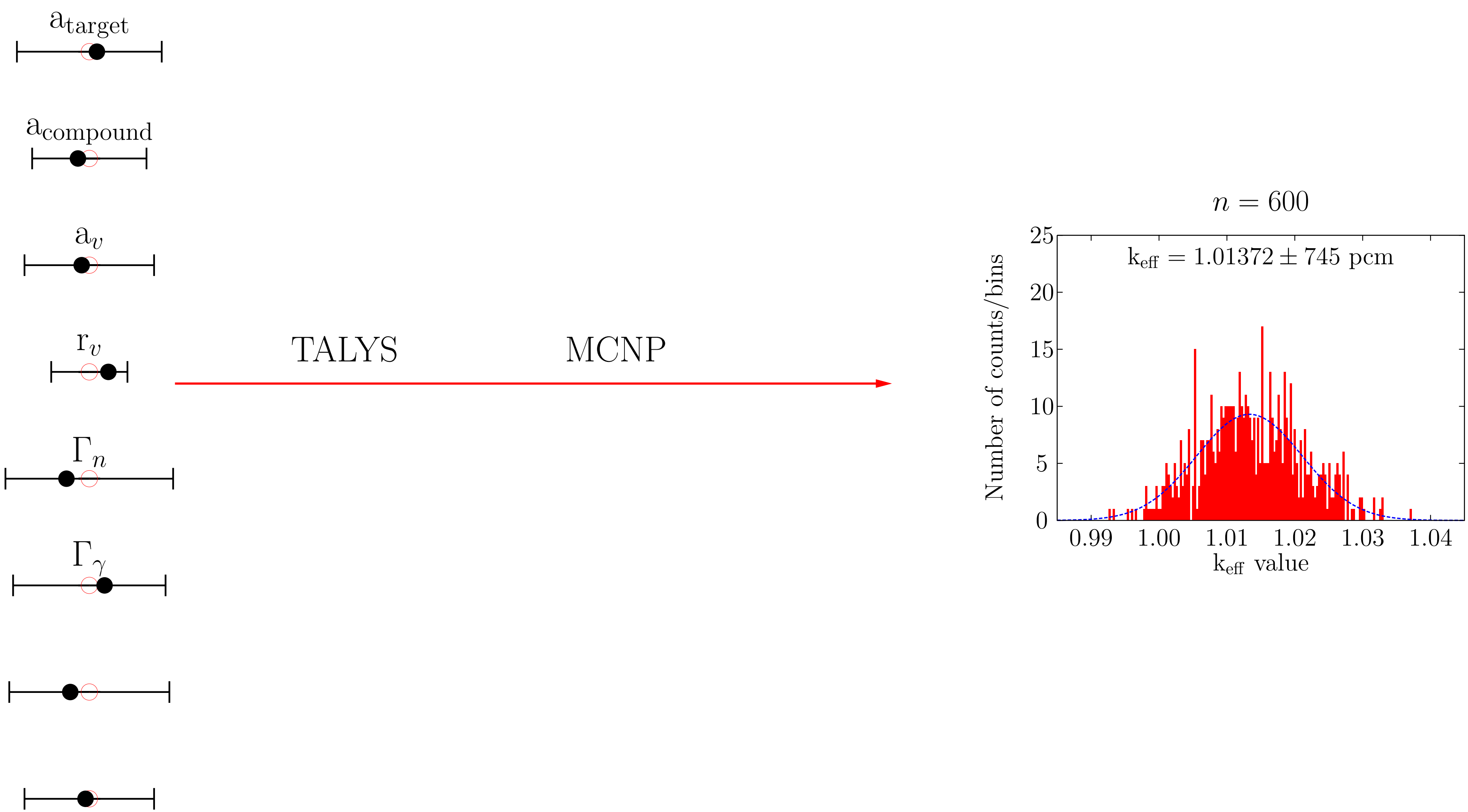

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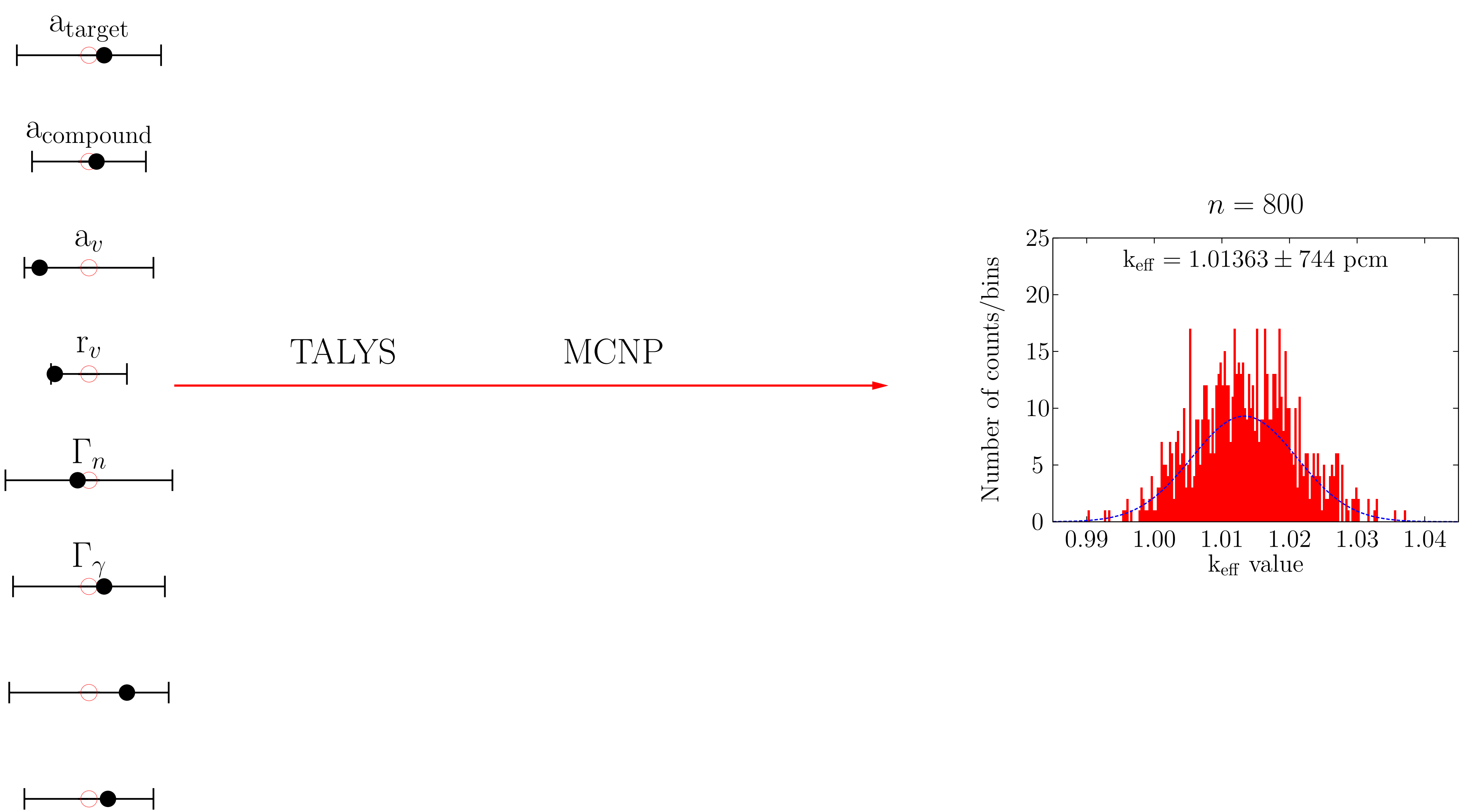

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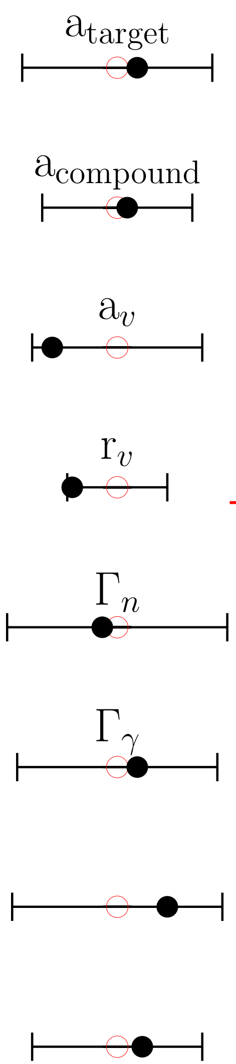
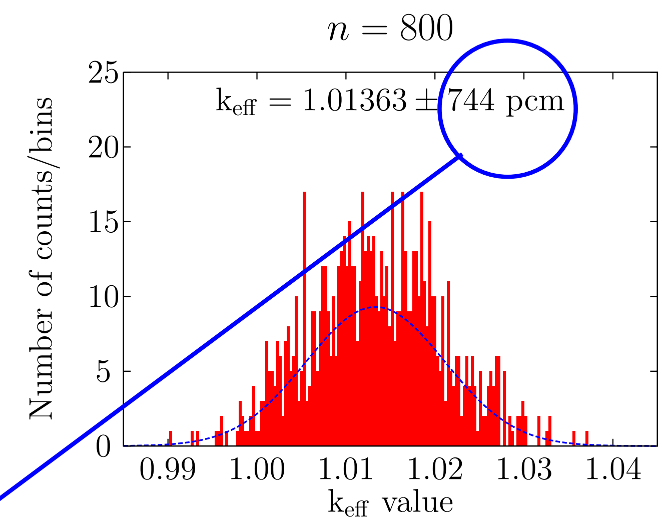



TALYS MCNP




Statistical uncertainty $\simeq$ 68 pcm

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

## Where can we apply it and examples with Pb isotopes

- ☞ Monte Carlo codes (MCNP, Tripoli), Deterministic codes (APOLLO, WIMS)
- ☞ Quantities: criticality, flux ( + all from SG-26), shielding and fusion

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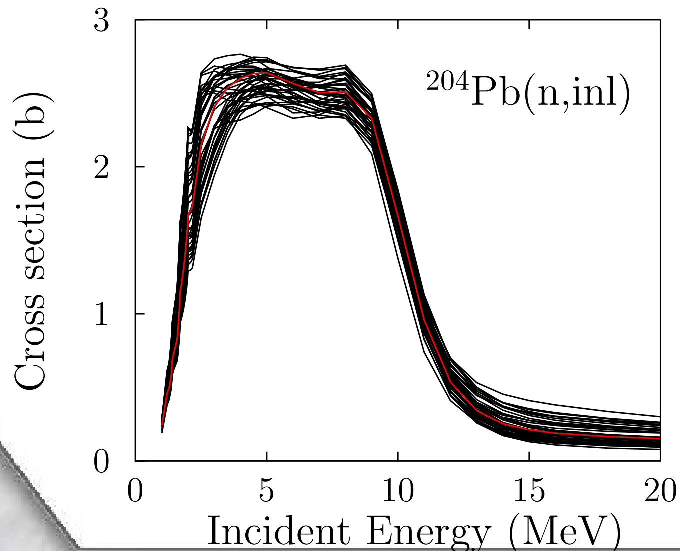
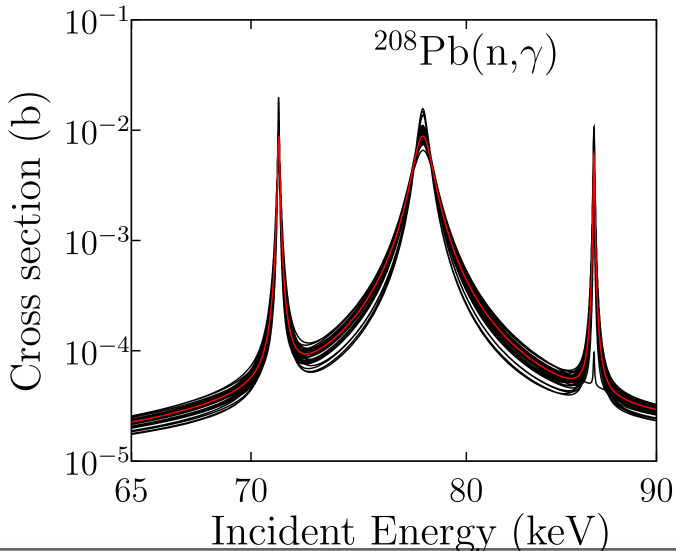
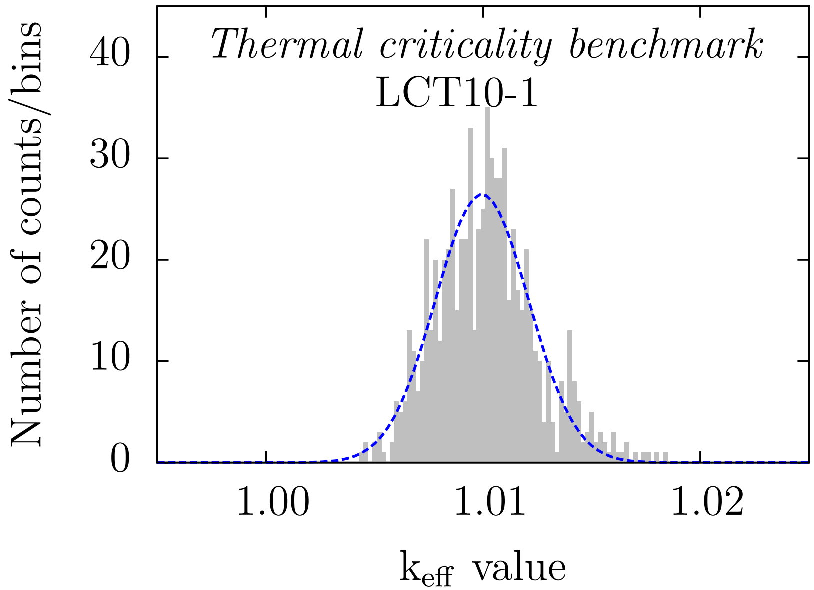
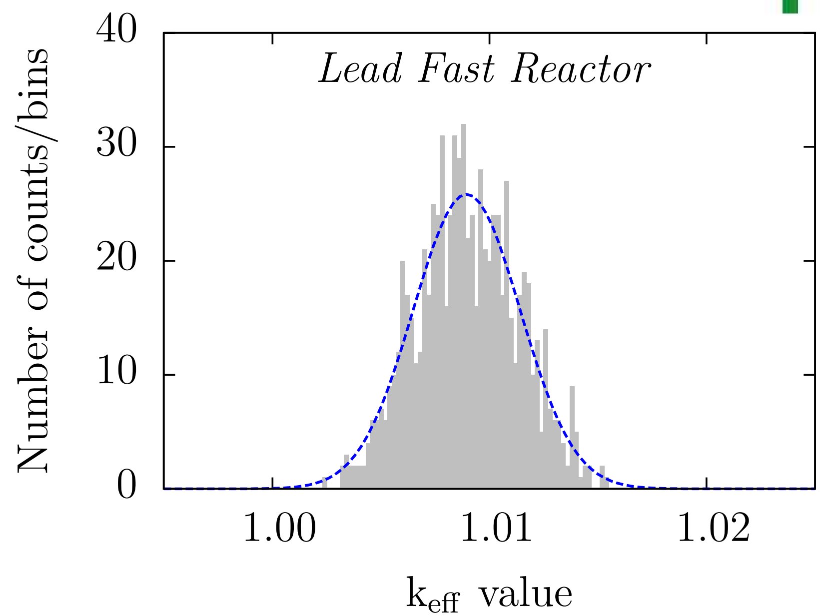
- $^{204-208}$Pb evaluations (NIM A589 (2008) 85) + **5000** random ENDF files
- Applied on $k_{eff}$ and $\beta_{eff}$ for criticality benchmarks (LCT-10 and HMF-64) and to ADS and LFR



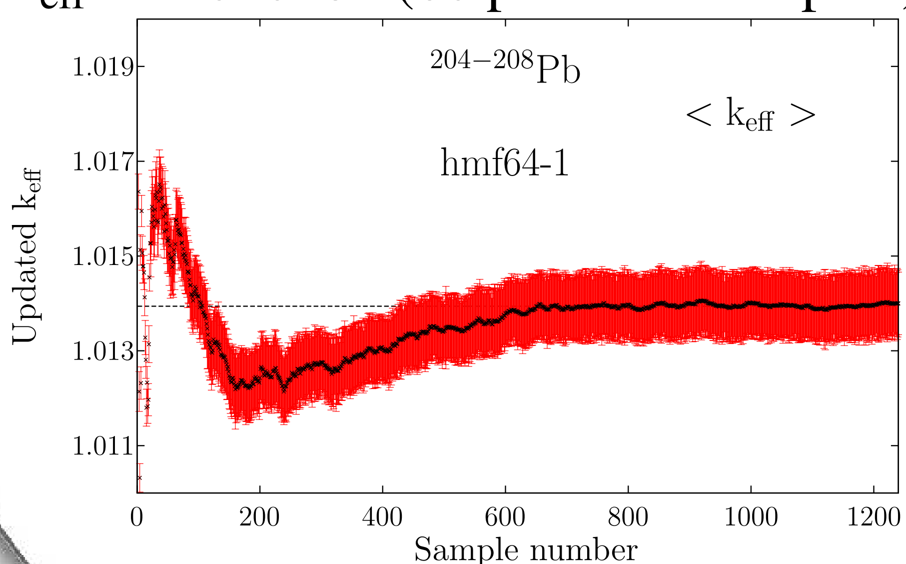
# Examples with Pb isotopes

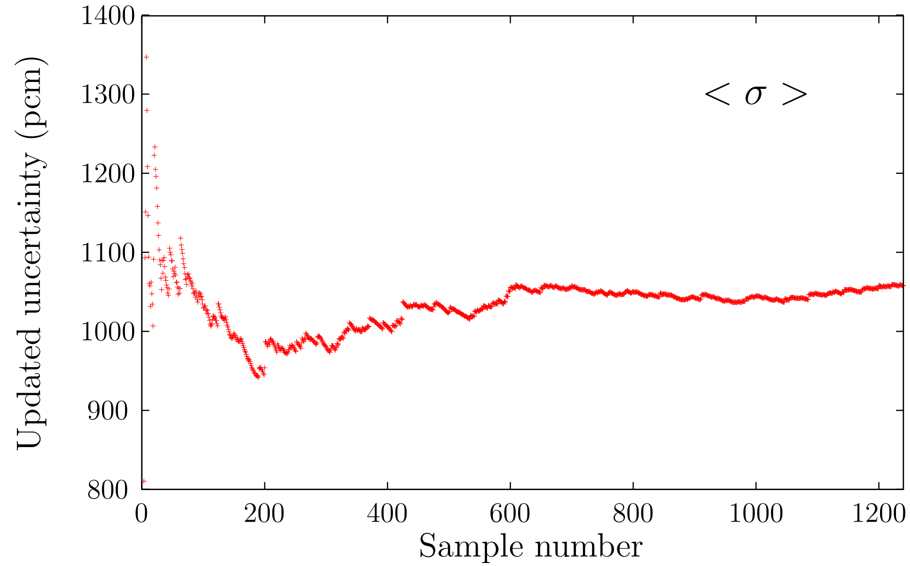



$k_{eff} = 1.01028 \pm (60$ pcm and $212$ pcm$)$

$k_{eff} = 1.00894 \pm (60$ pcm and $240$ pcm$)$



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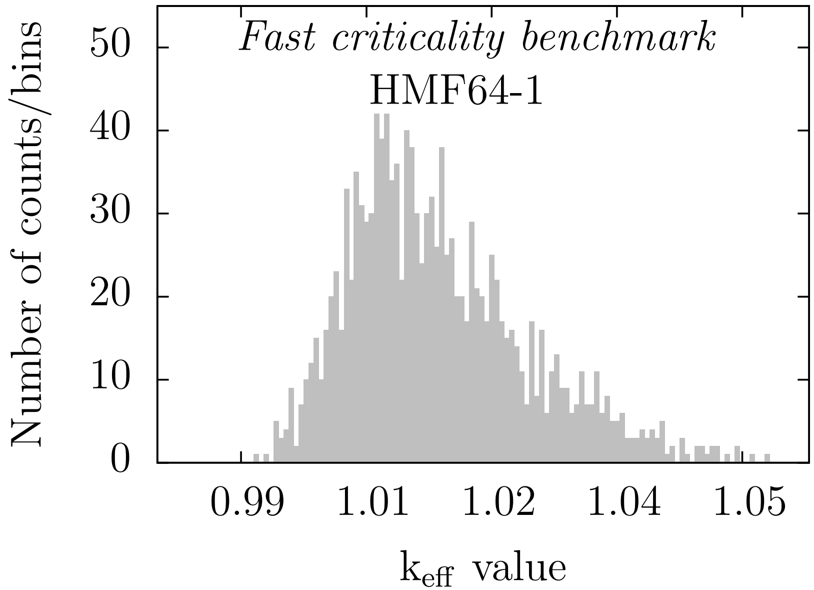


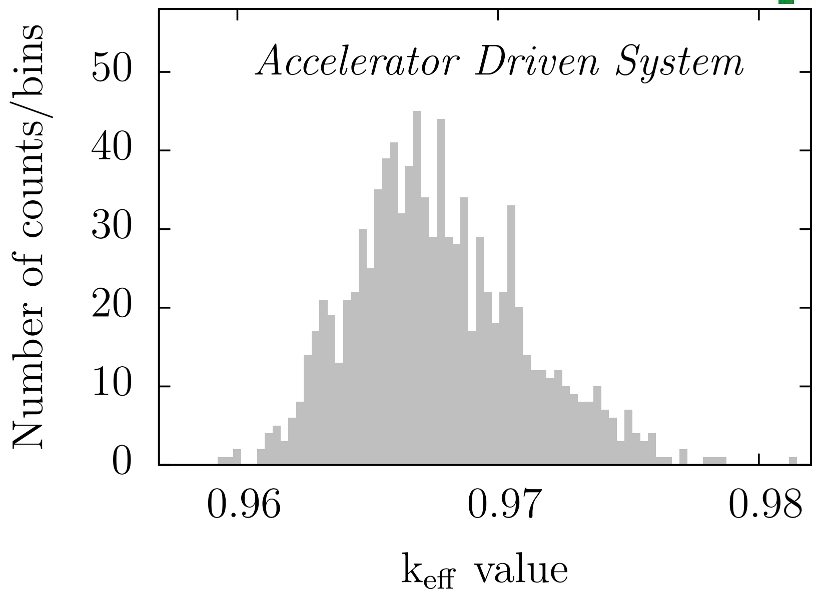

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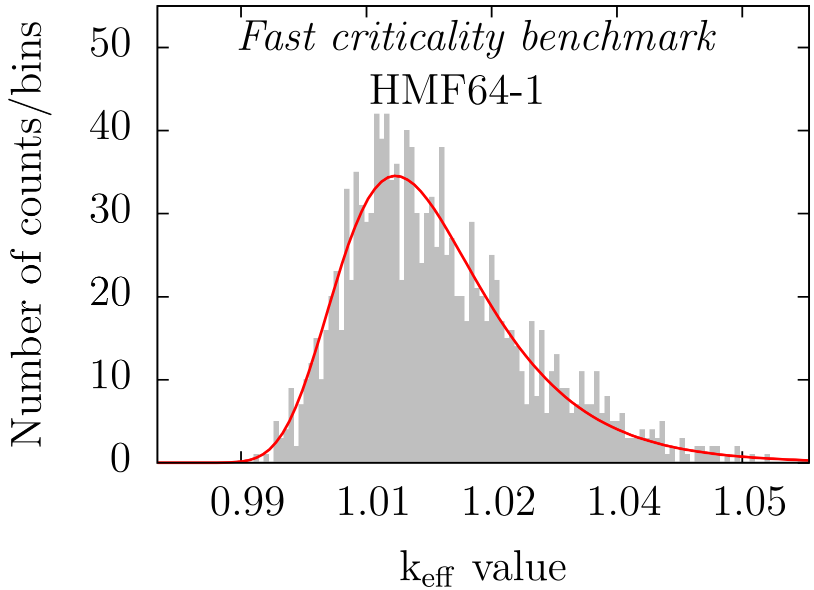


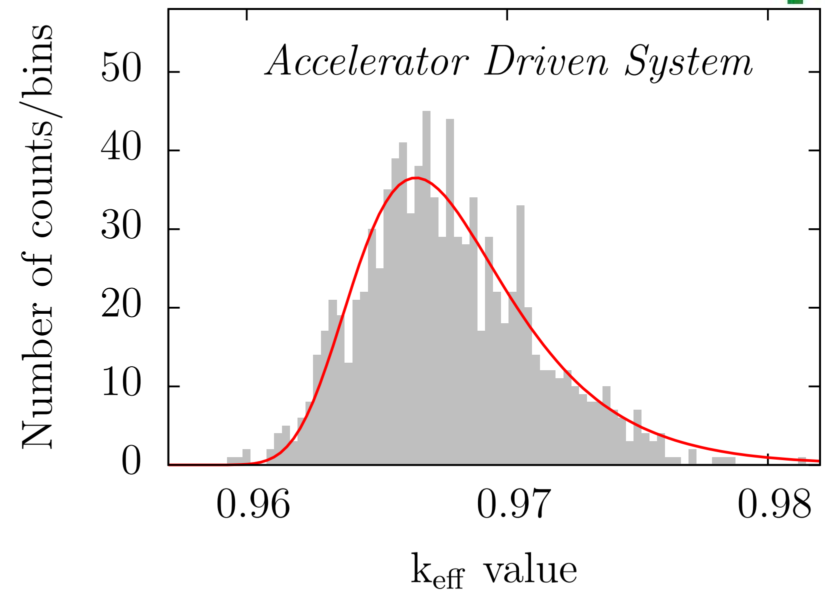


Better fit with the "*Extreme Value Theory*", or EVT:

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

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

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

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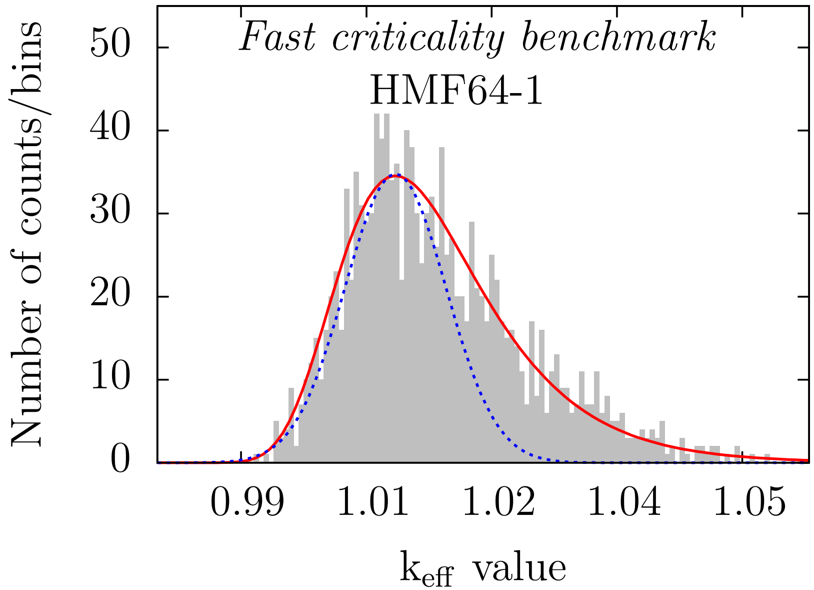


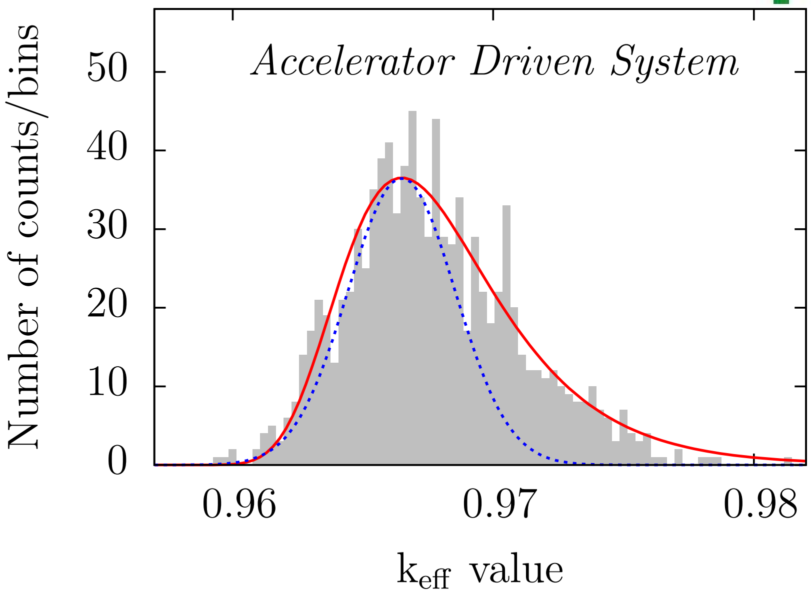


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| | HMF-64.1 | ADS |
|---|---|---|
| $k_{eff}$ | 1.00848<br>$\mu'$=1.01394 | 0.96648<br>$\mu'$=0.96785 |
| $\sigma_k \times 10^5$ | **855**<br>**$\sigma'$=1097** | **291**<br>**$\sigma'$=345** |

## Global calculations: from $^{12}$C to $^{240}$Pu

*"In general, this paper will or will not be a breakthrough in methodology if the [practicality and robustness] can or can not be demonstrated."*,

ANE Referee, May 2008

*"What about actinides, what about real systems ?"*,

JEFF &WPEC meetings, May-June 2008

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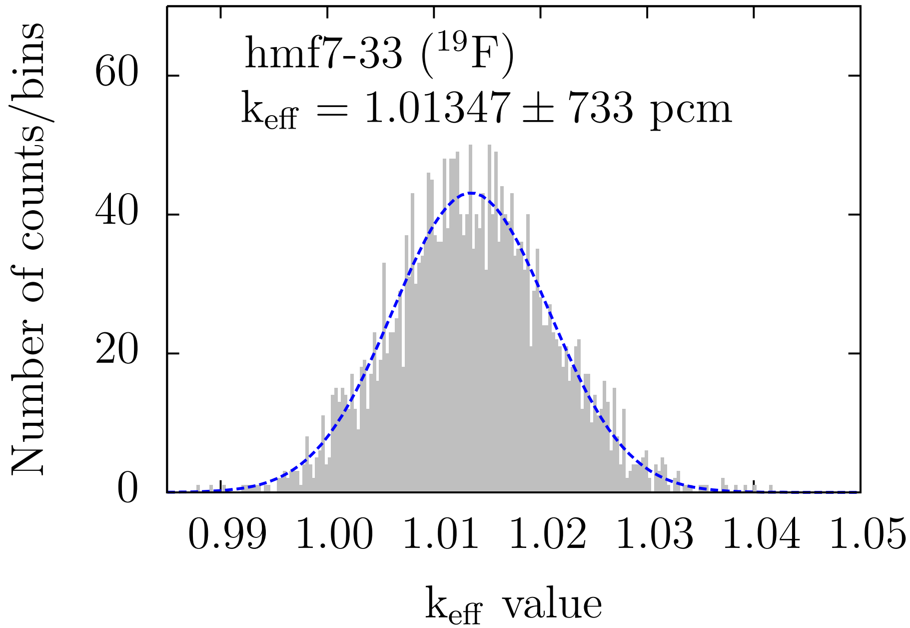
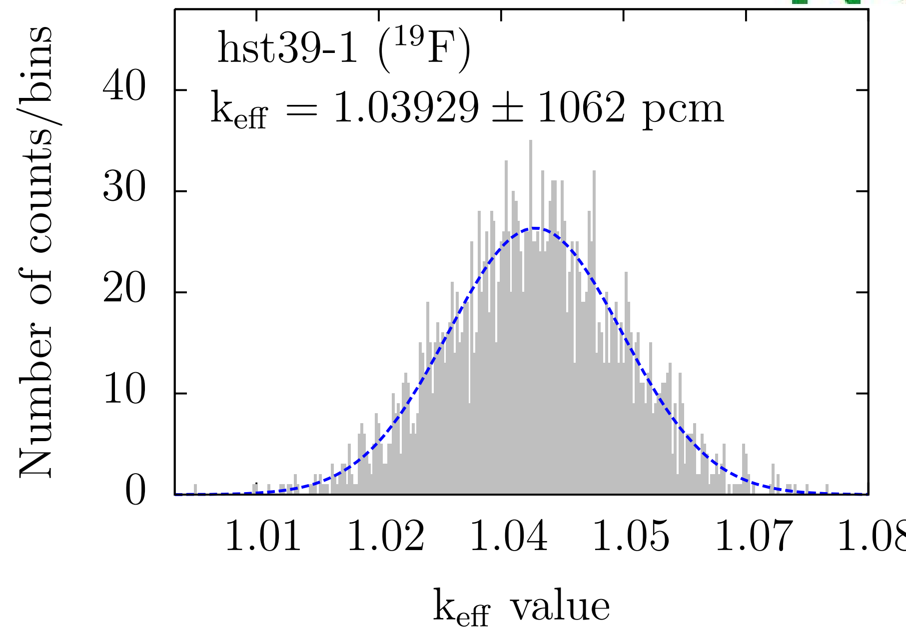
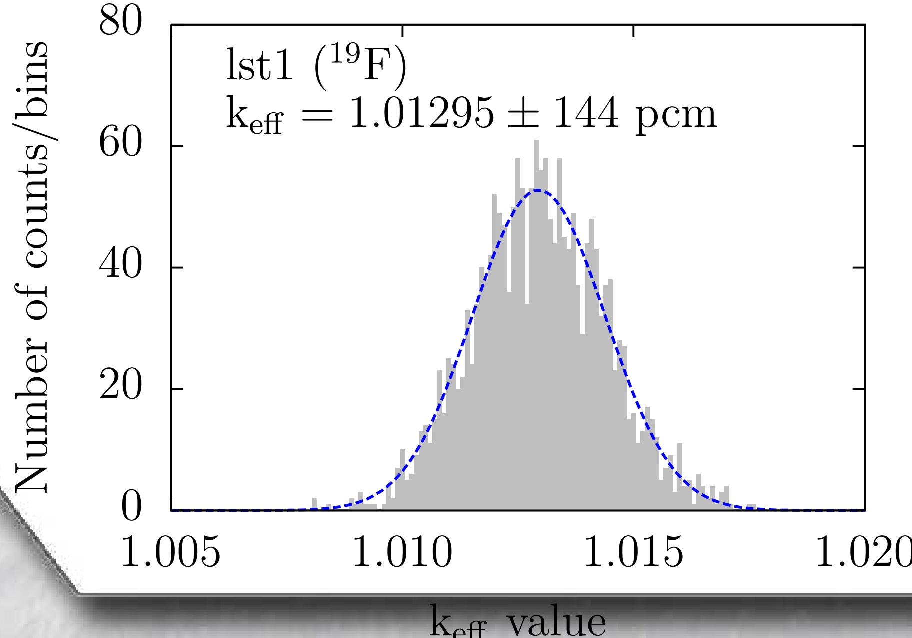
Okay, let's go from academic solutions (☕) to mass/applied production (🏭) !

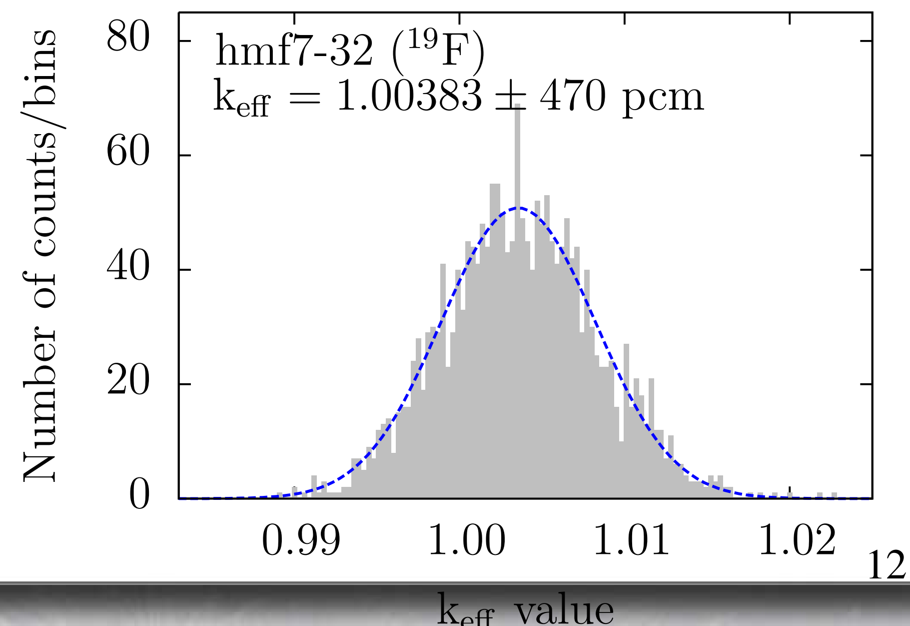
- Default TALYS calculation + Resonance parameters (RP) + uncertainties
- 100 to 2000 ENDF files per isotope from $^{12}$C to $^{240}$Pu ($\simeq$ 100 isotopes)
- 190 criticality-safety benchmarks ($>$ 60 000 calculations) from the ICSBP
- All Oktavian shielding benchmarks (neutrons and gammas)
- Reactivity swing for a LWR using an "Inert Matrix Fuel" (Pu and Mo)
- $k_{eff}$ for a HTR (PBMR), ESKOM specifications

# Examples of $k_{eff}$ benchmarks for $^{19}F$

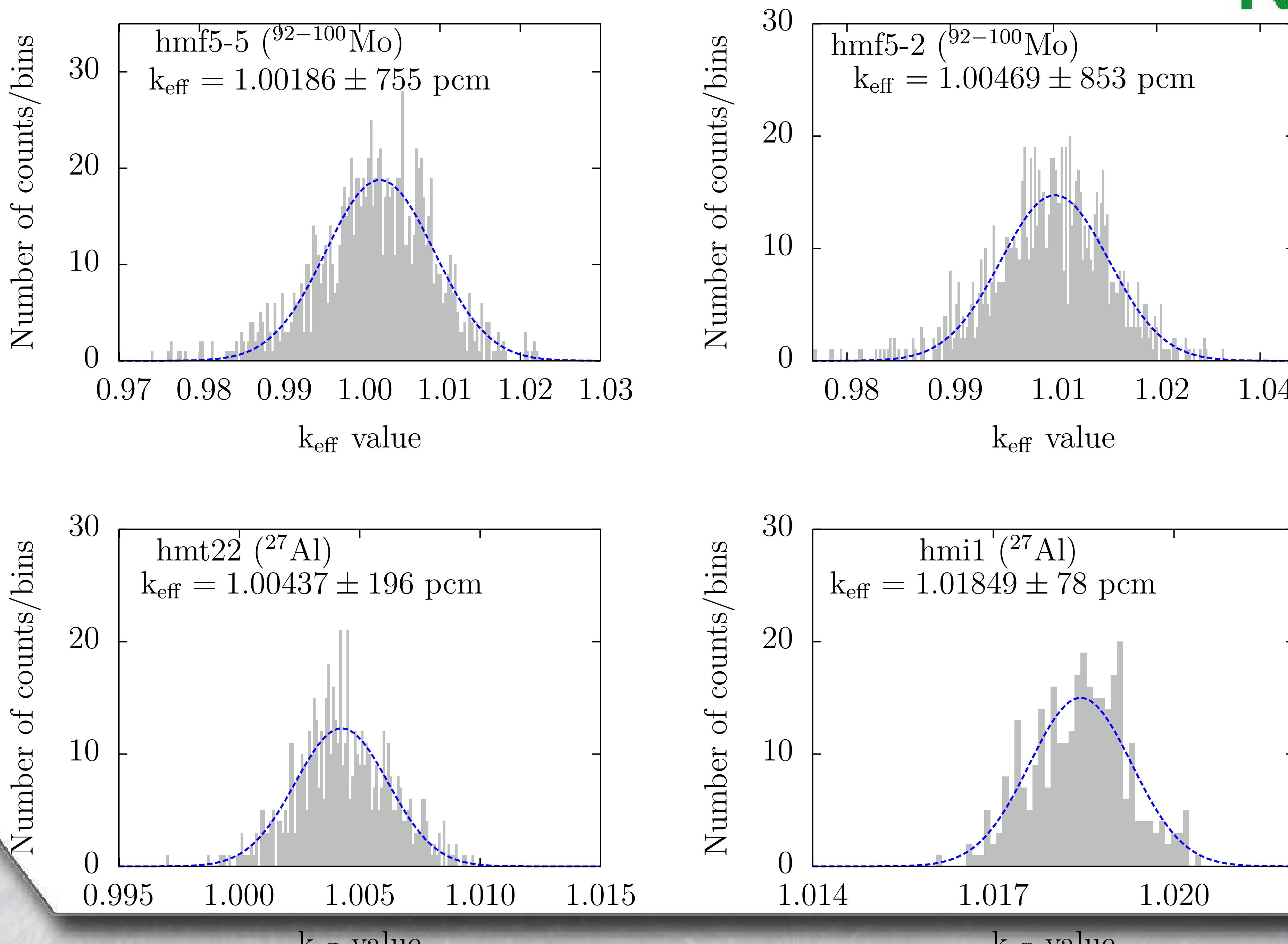


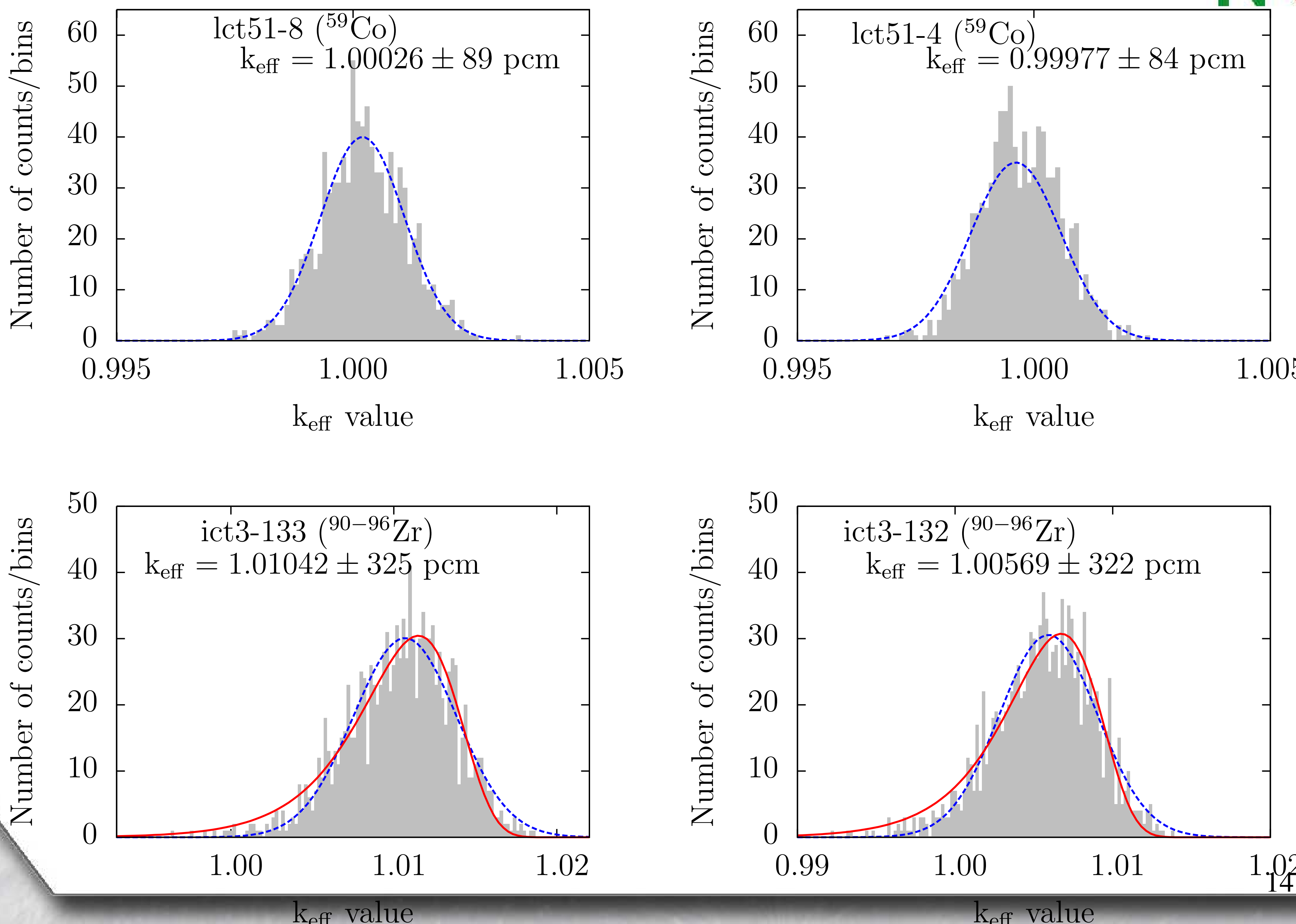



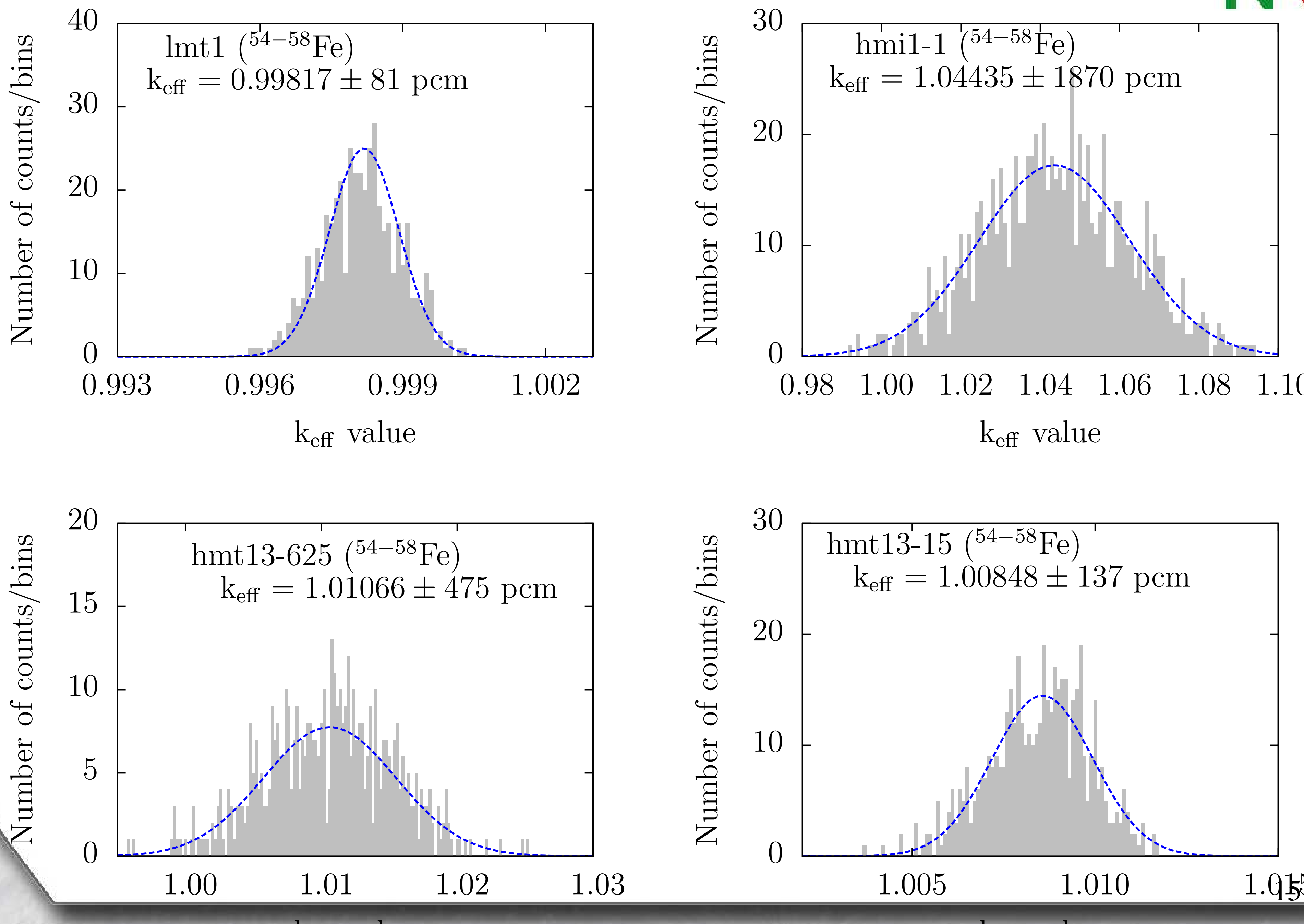
# Examples of $k_{eff}$ benchmarks for $^{27}$Al and $^{92-100}$Mo



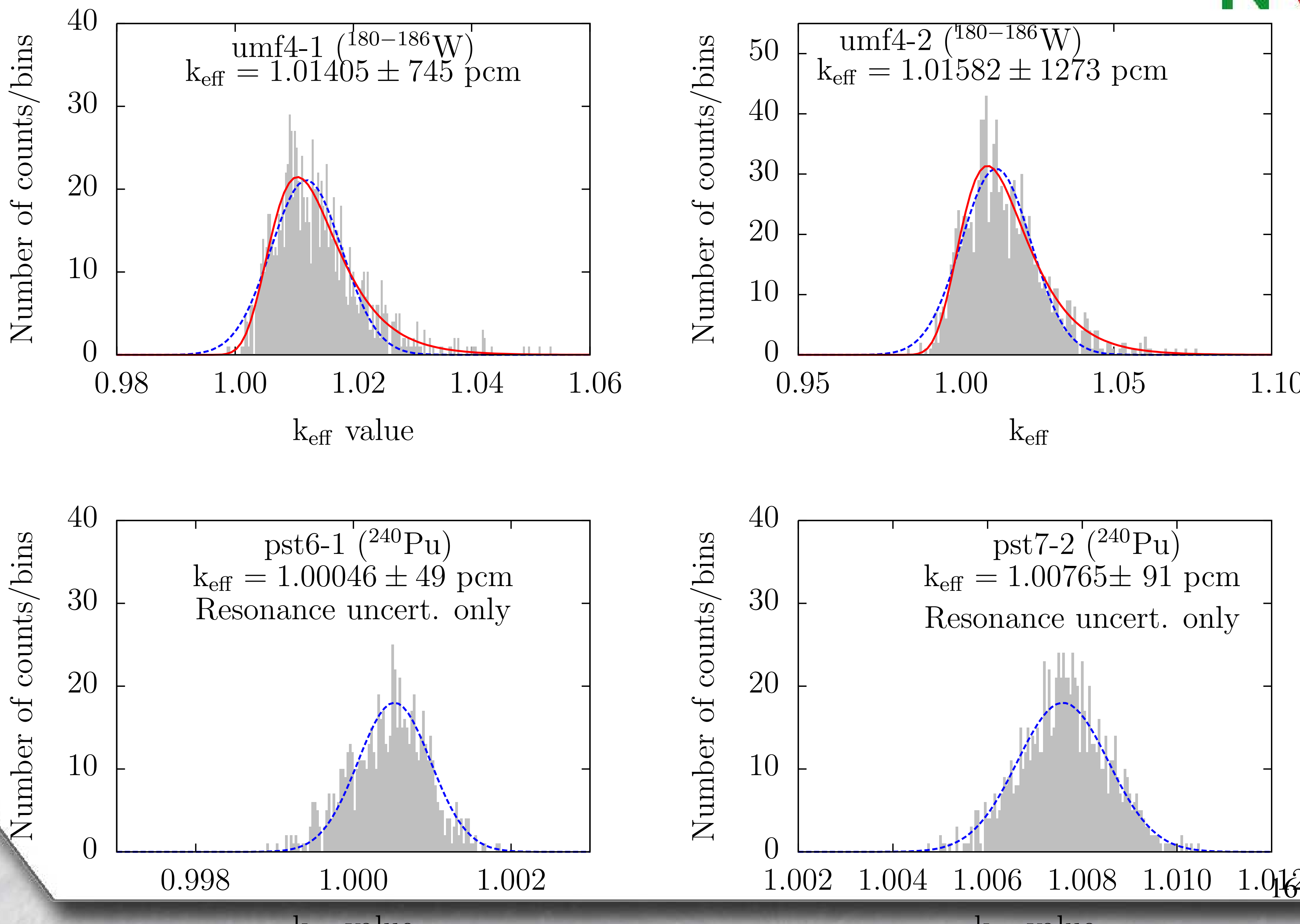
# Examples of $k_{eff}$ benchmarks for $^{59}$Co and $^{90-96}$Zr



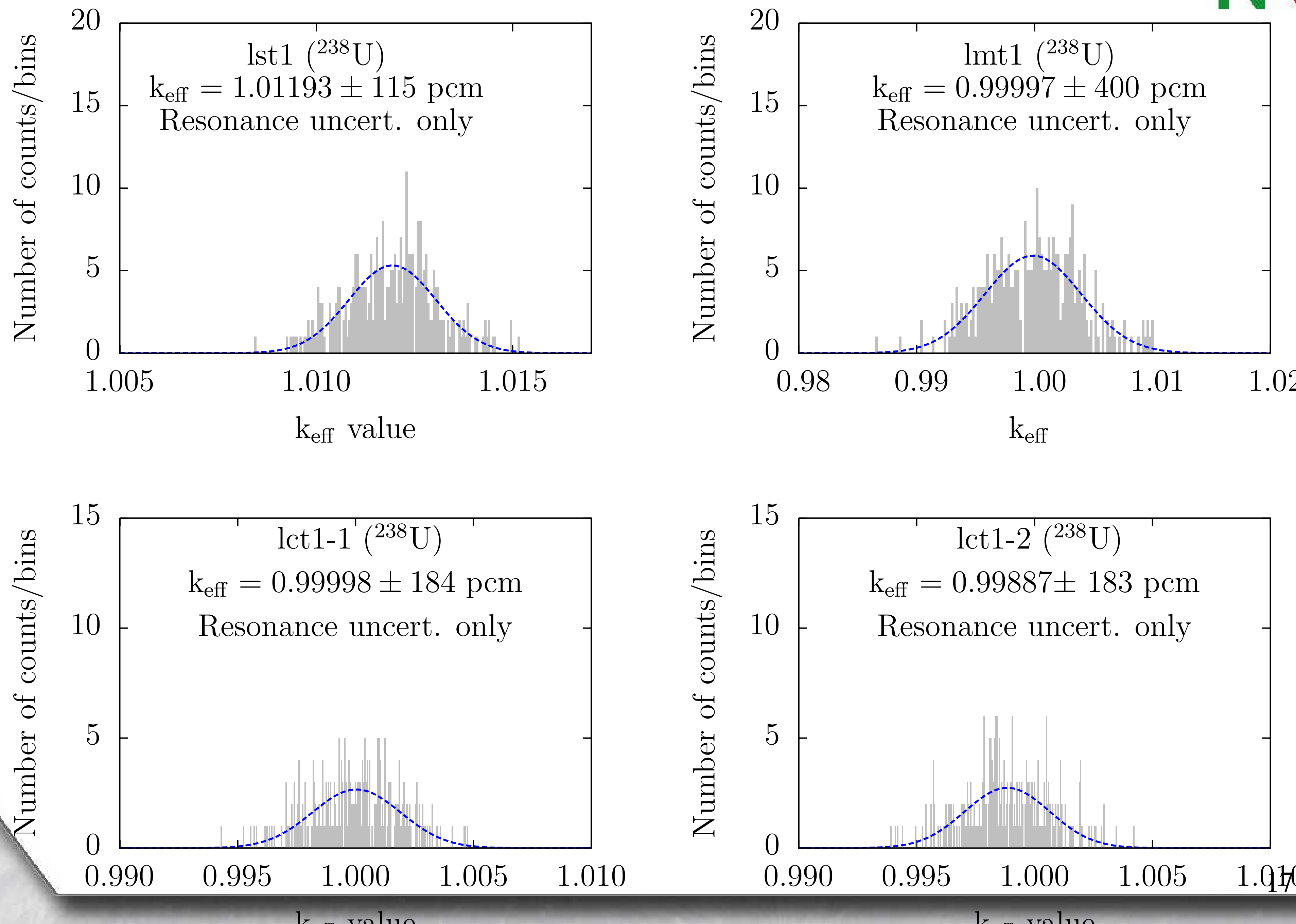
# Examples of $k_{eff}$ benchmarks for $^{54-58}$Fe



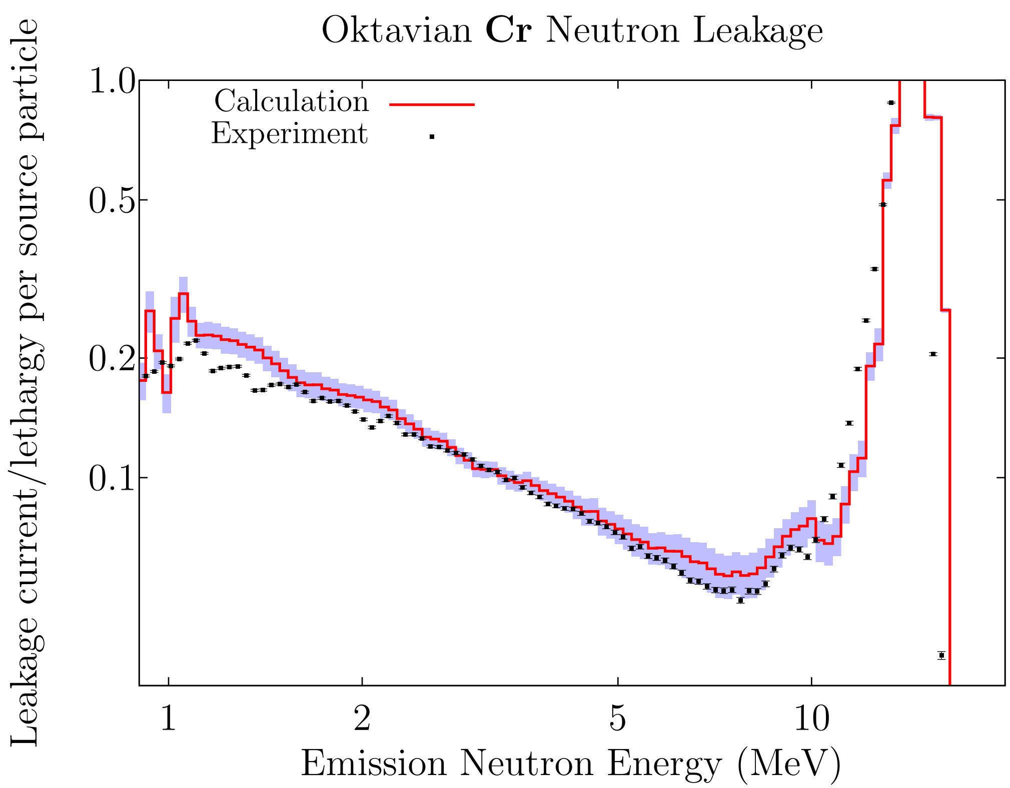
# Examples of $k_{eff}$ benchmarks for $^{180-186}$W and $^{240}$Pu

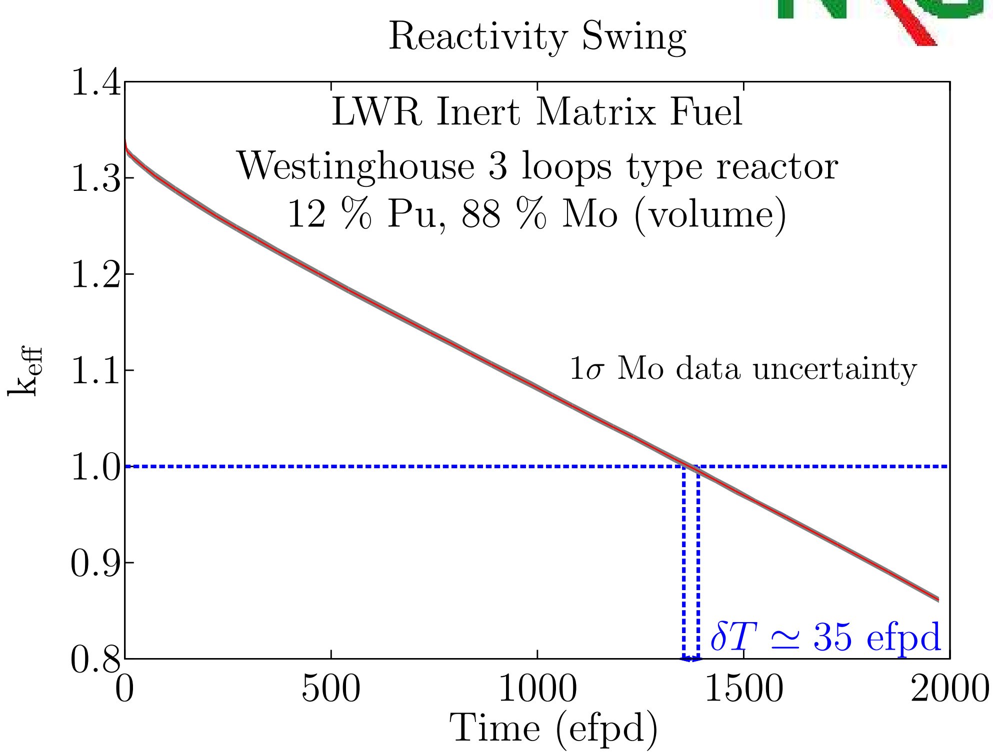


# Examples of $k_{eff}$ benchmarks for $^{238}$U



# Examples of shielding benchmarks and reactivity swing



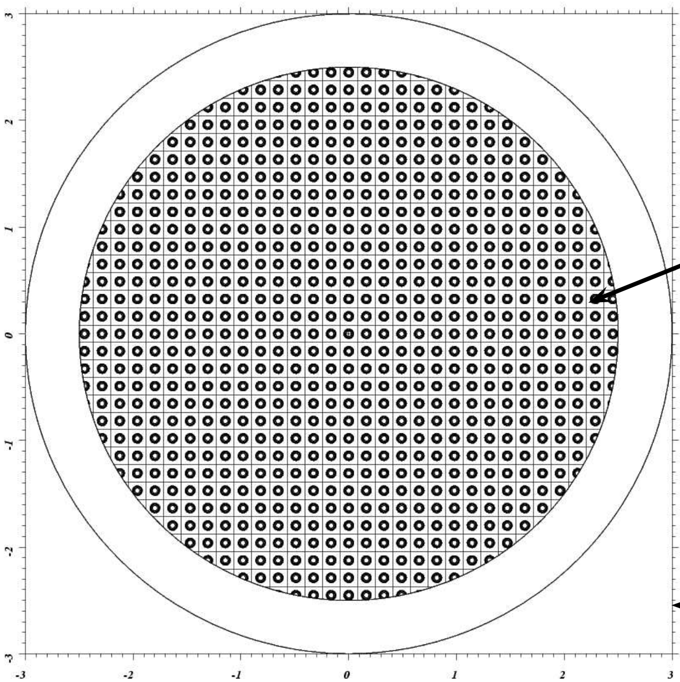




(Blind Talys calculations)

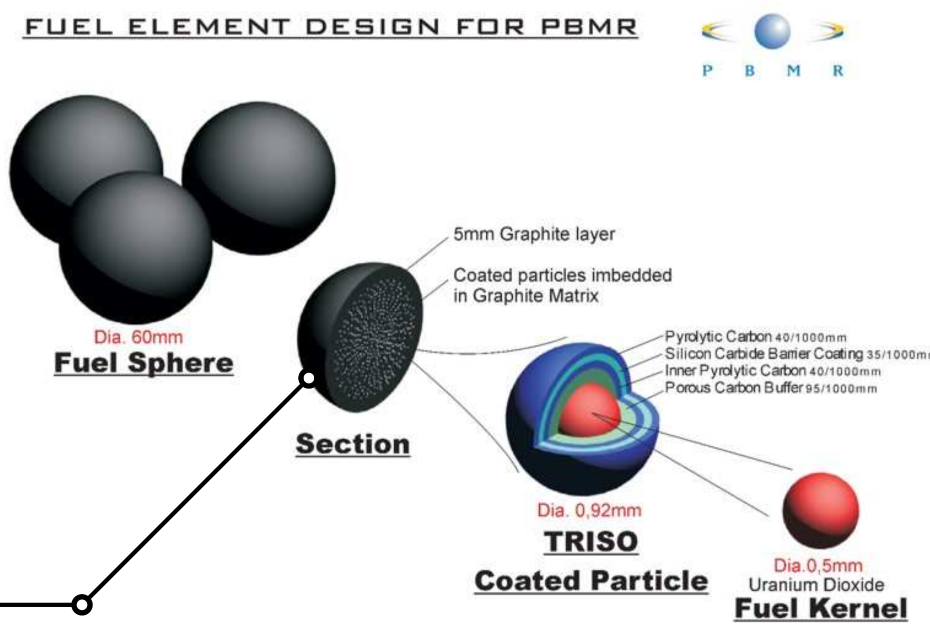
- Also applied to Mn, Co, Al, Cu Oktavian benchmarks
- and industrial PWR reactor for life-time extension (uncertainty on the reactor pressure vessel damage)

# Application to a Pebble Bed Modular Reactor (PBMR)

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



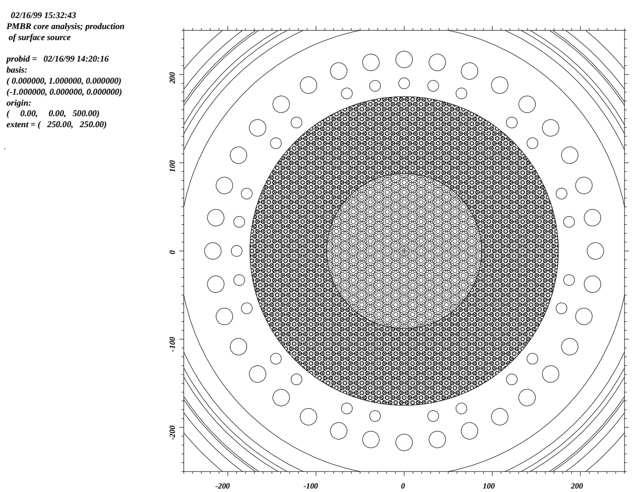

0.5 mm

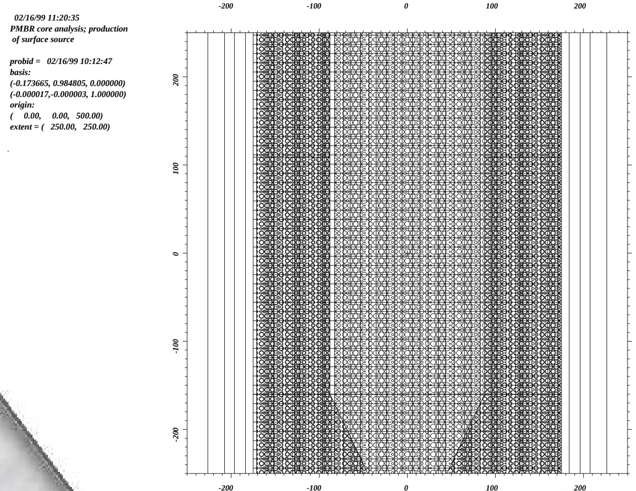


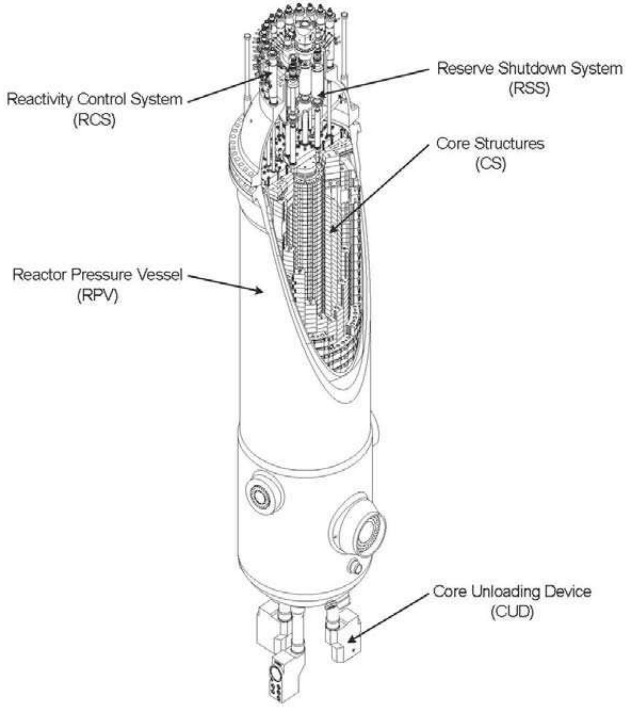

6 cm

# Application to a Pebble Bed Modular Reactor (PBMR)

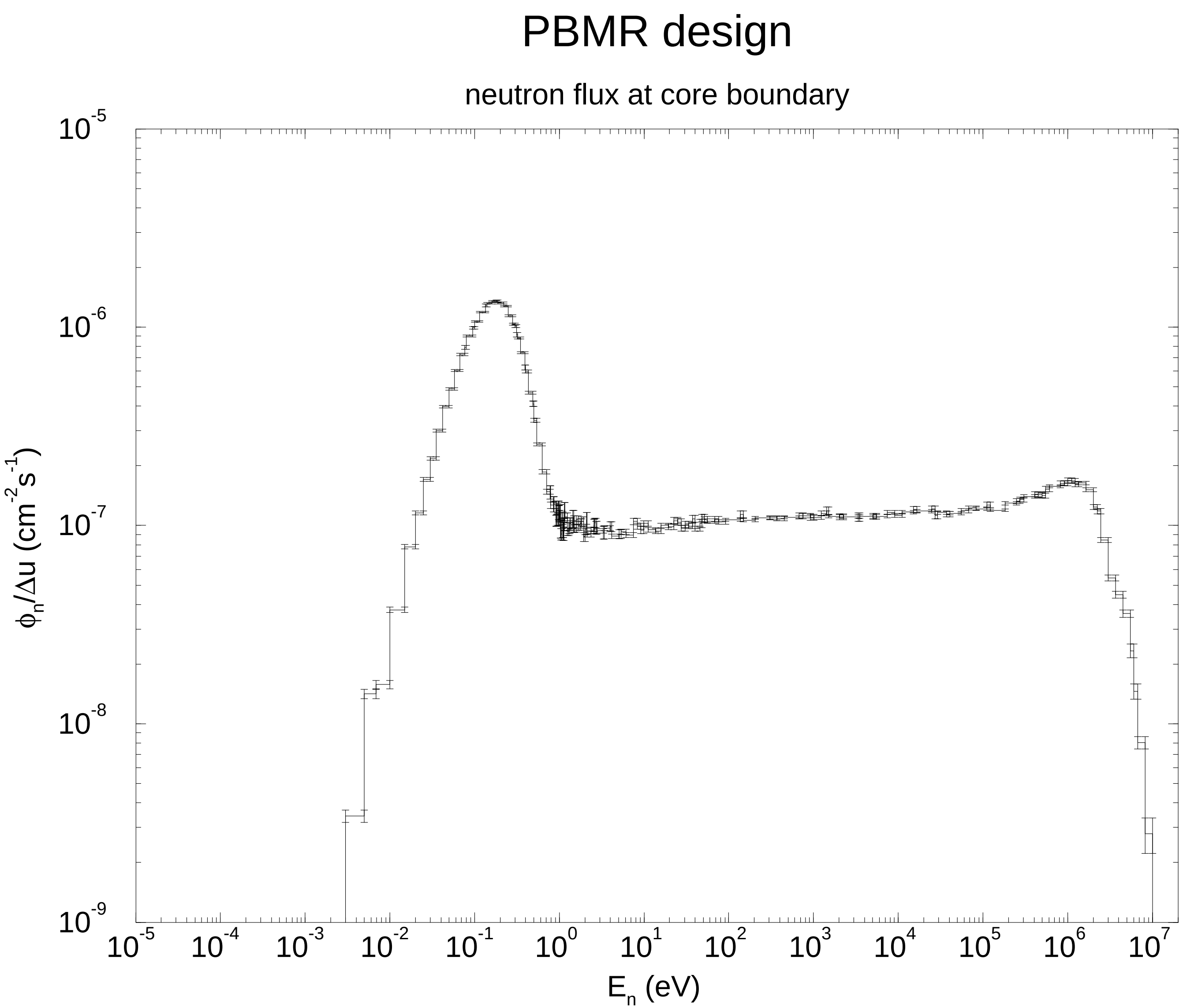
- Hexagonal close packed lattice
- Moderator region consists of homogeneous moderator pebbles as the fuel, reflectors and shields as defined by ESKOM



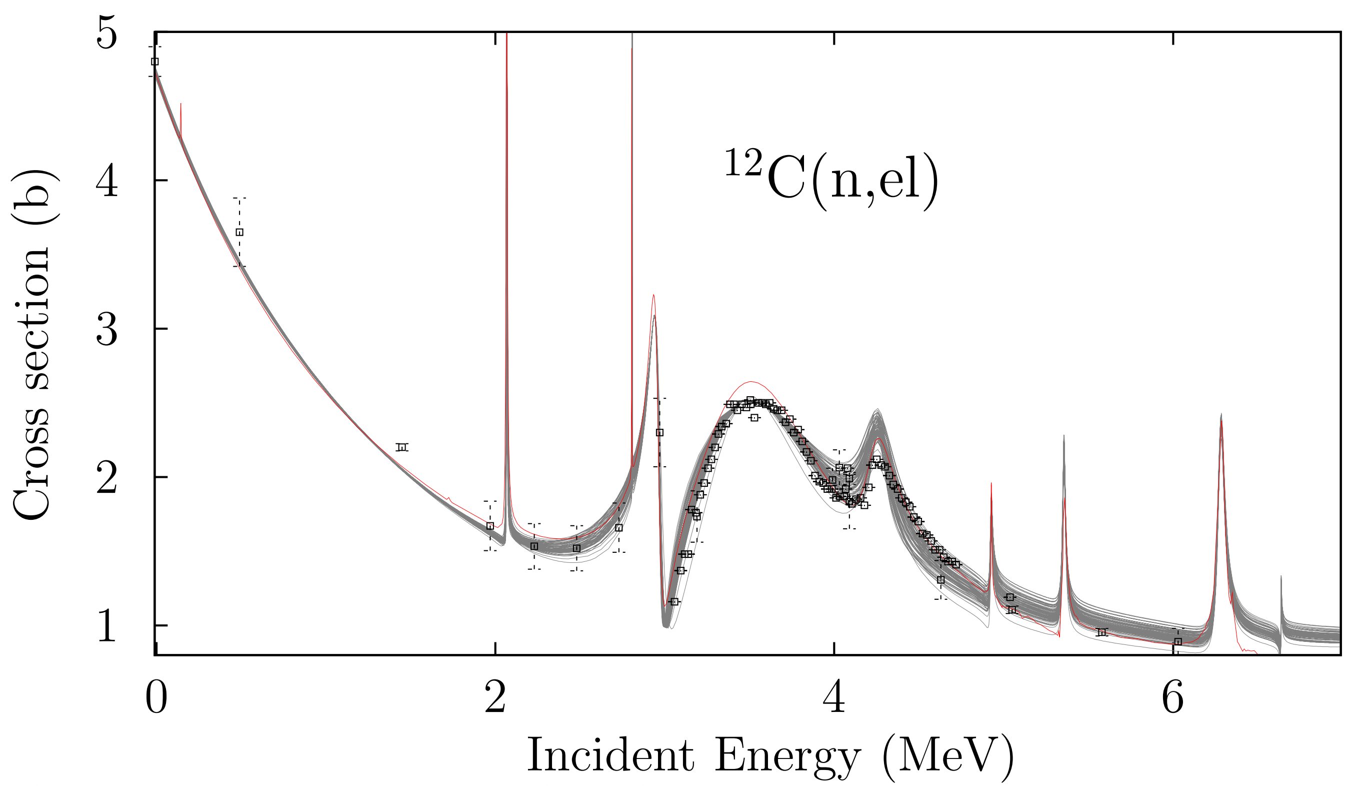
# PBMR: Neutron Flux spectrum



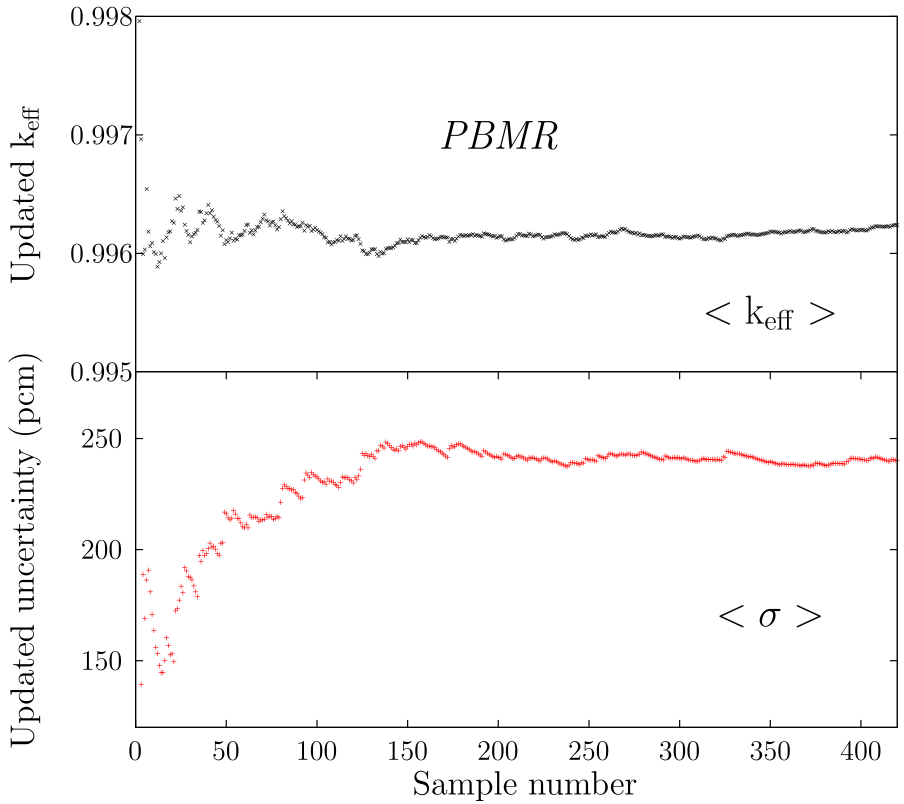

Neutron flux spectrum at the radial core boundary (Almost no neutron above few MeV)

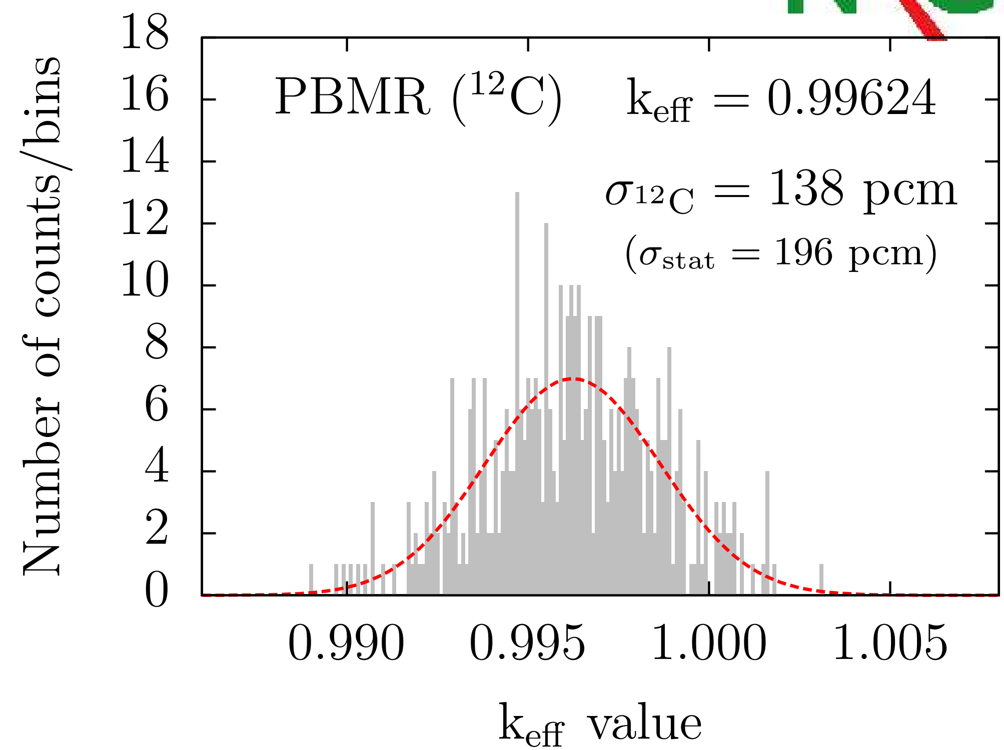
## PBMR: $^{12}C$ nuclear data

- For neutron energy lower than few MeV: only elastic and capture cross sections
- JEFF-3.1: $\sigma_{th}$ (n,el)$= 4.746 \pm 0.002$b and $\sigma_{th}$ (n,$\gamma$)$= 3.53 \pm 0.07$mb
- All (n,el), (n,$\gamma$), 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)

## Pros and Cons

- ☺ + No MF 32-35 (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
- ☺ + QA
- ☹ - Needs discipline to reproduce
- ☹ - Memory and computer time
- ☹ - Complexity for full reactor core calculation not fully investigated
- ☹ - Role of data centers would change

## Conclusions and future improvements

- ✗ New methodology to propagate nuclear data uncertainty to integral quantities ($k_{eff}$ benchmarks, shielding benchmarks, reactivity swing, neutron flux for commercial reactor) via Monte Carlo
- ✗ Proof of principle with high quality Pb evaluations
- ✗ Mass production tested on more than 190 benchmarks
- ✗ “Paper to present the principle”: under revision for ANE
- ✗ “Application to a real complex system”: PBMR
- □ Needs for better sampling in the resonance region
- □ Needs for a better “accept-reject” mechanism
- □ What if nuclear modeling does not match the accuracy of the measurements ? (how to sample ?)
- □ Needs to develop best central-value evaluations (non-fissile and fissile) ?