Living without covariance files

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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

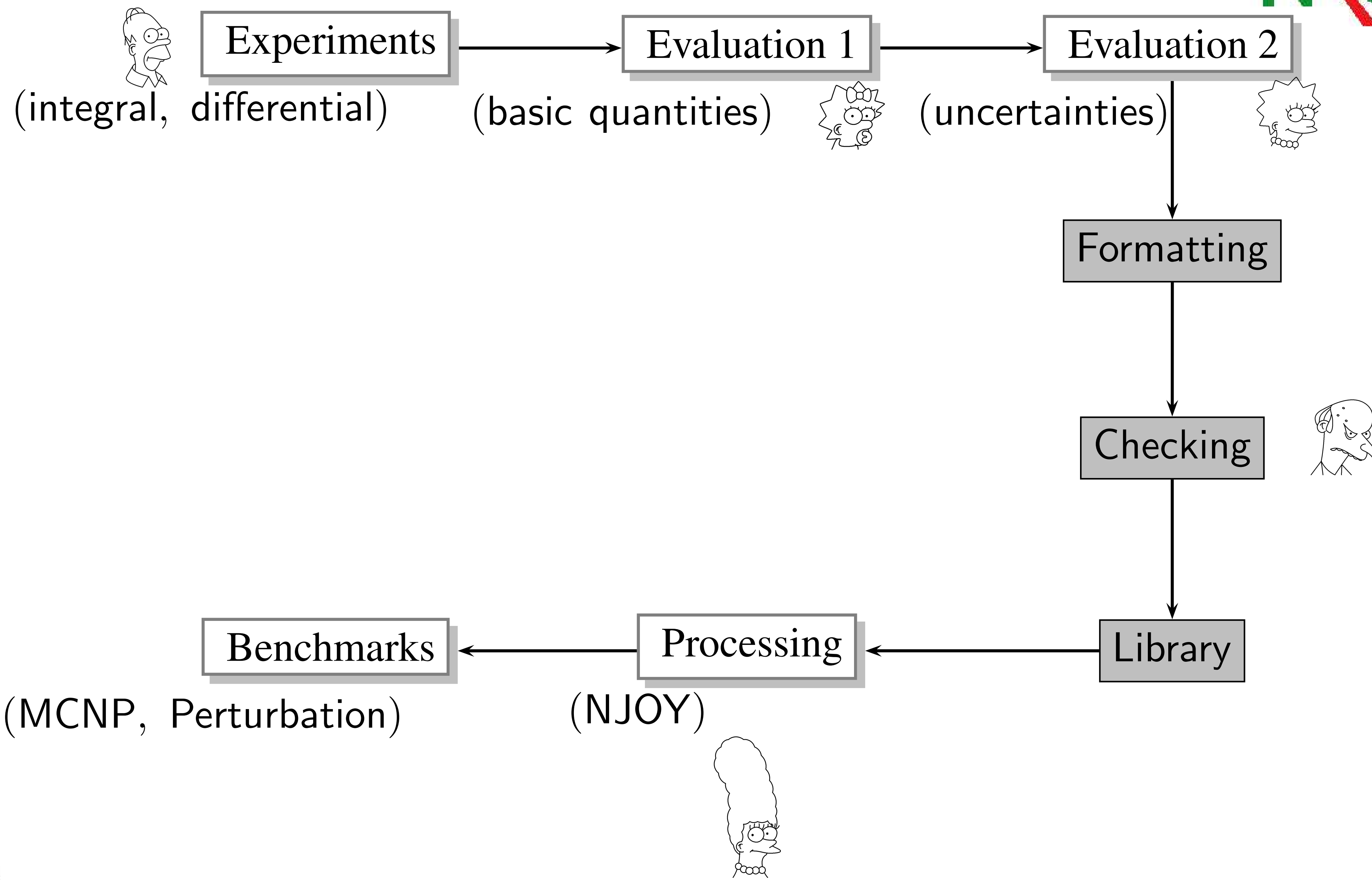
$\Longrightarrow$ Most straightforward way: Total Monte Carlo Approach !

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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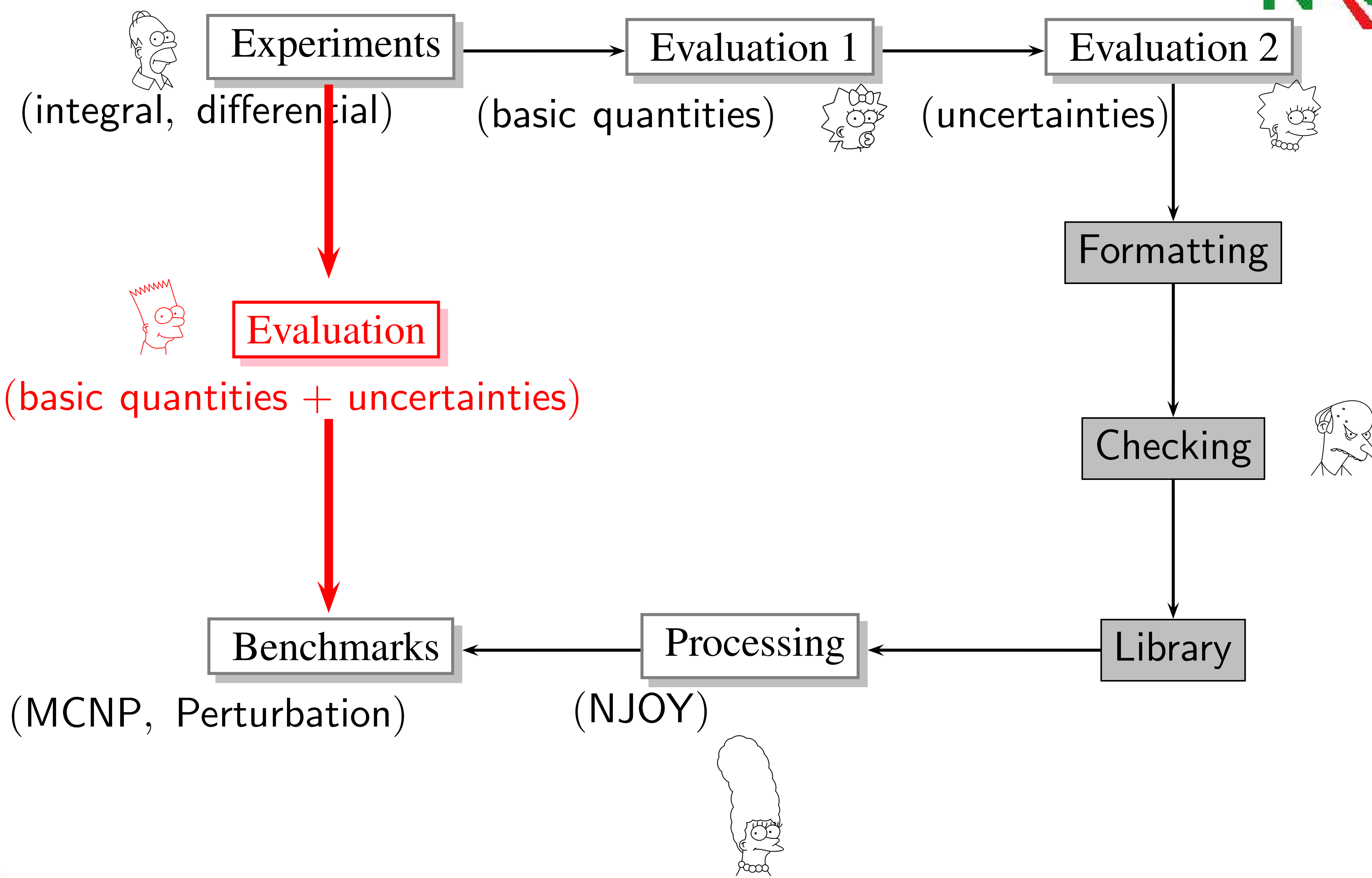

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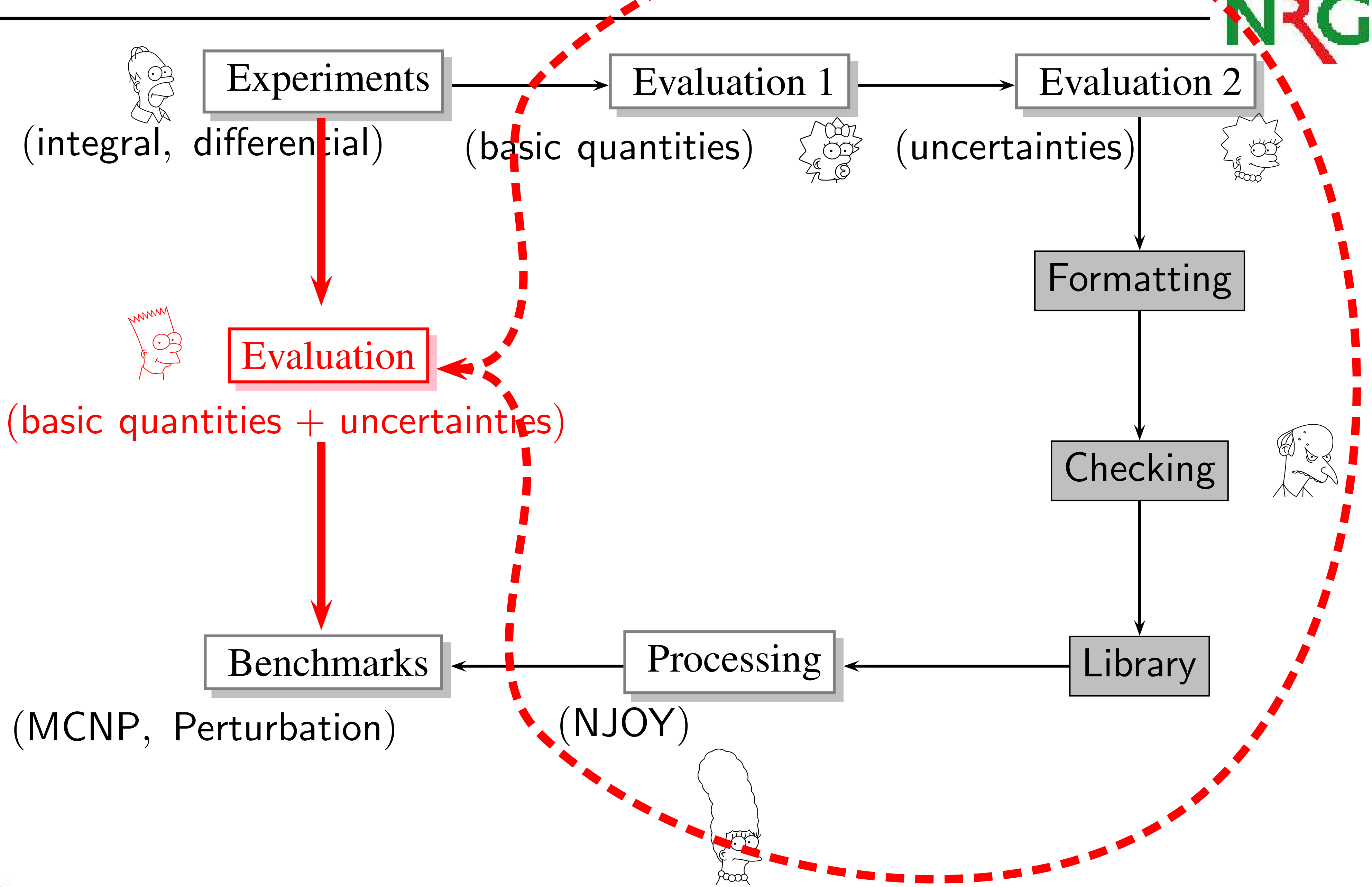
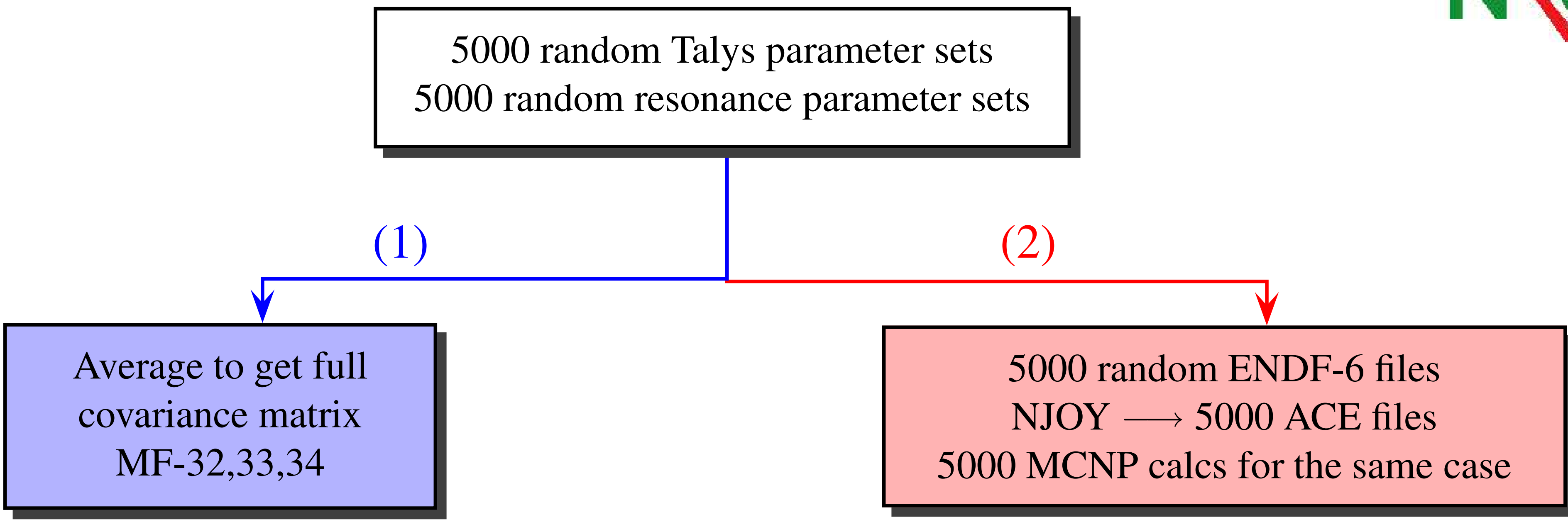


New (and most simple) path



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

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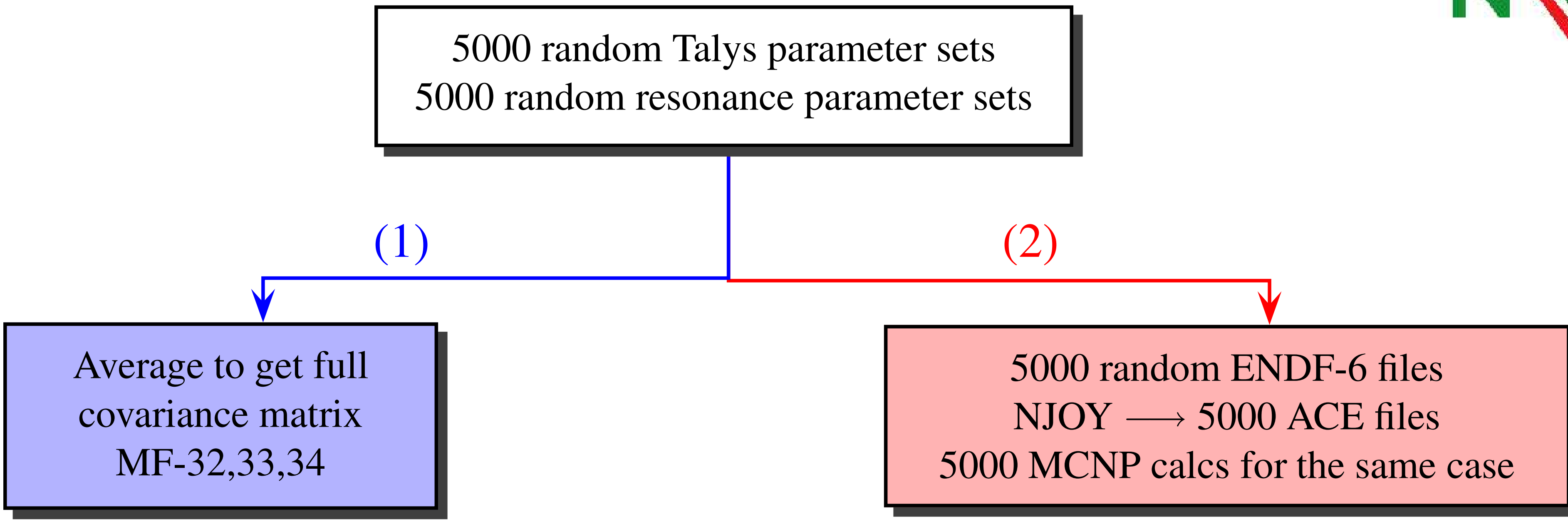


We have both routes, but one is easier and more exact to take than the second one.

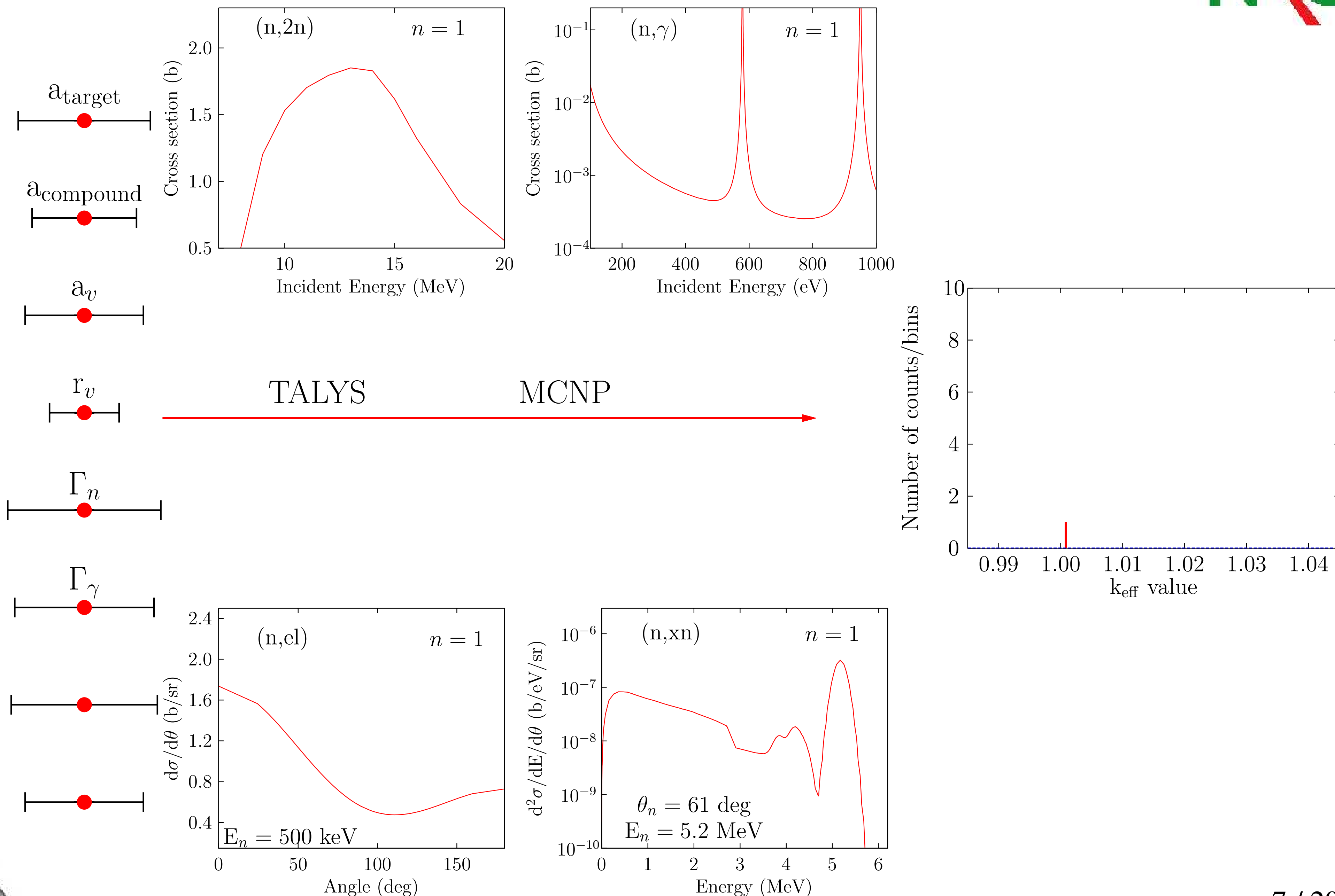
In solution (1):

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

Problem 2: Processing of these covariances

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

Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



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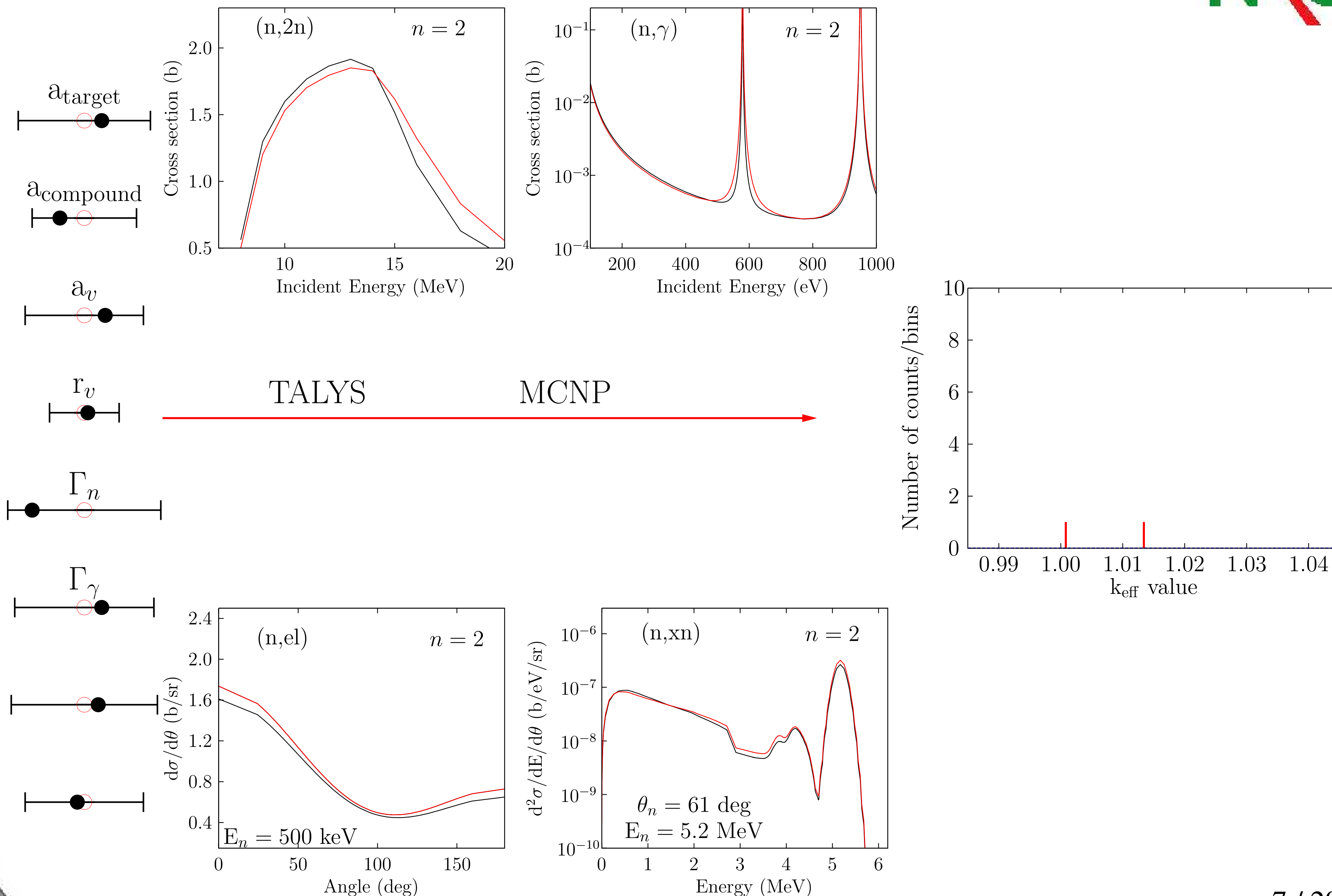

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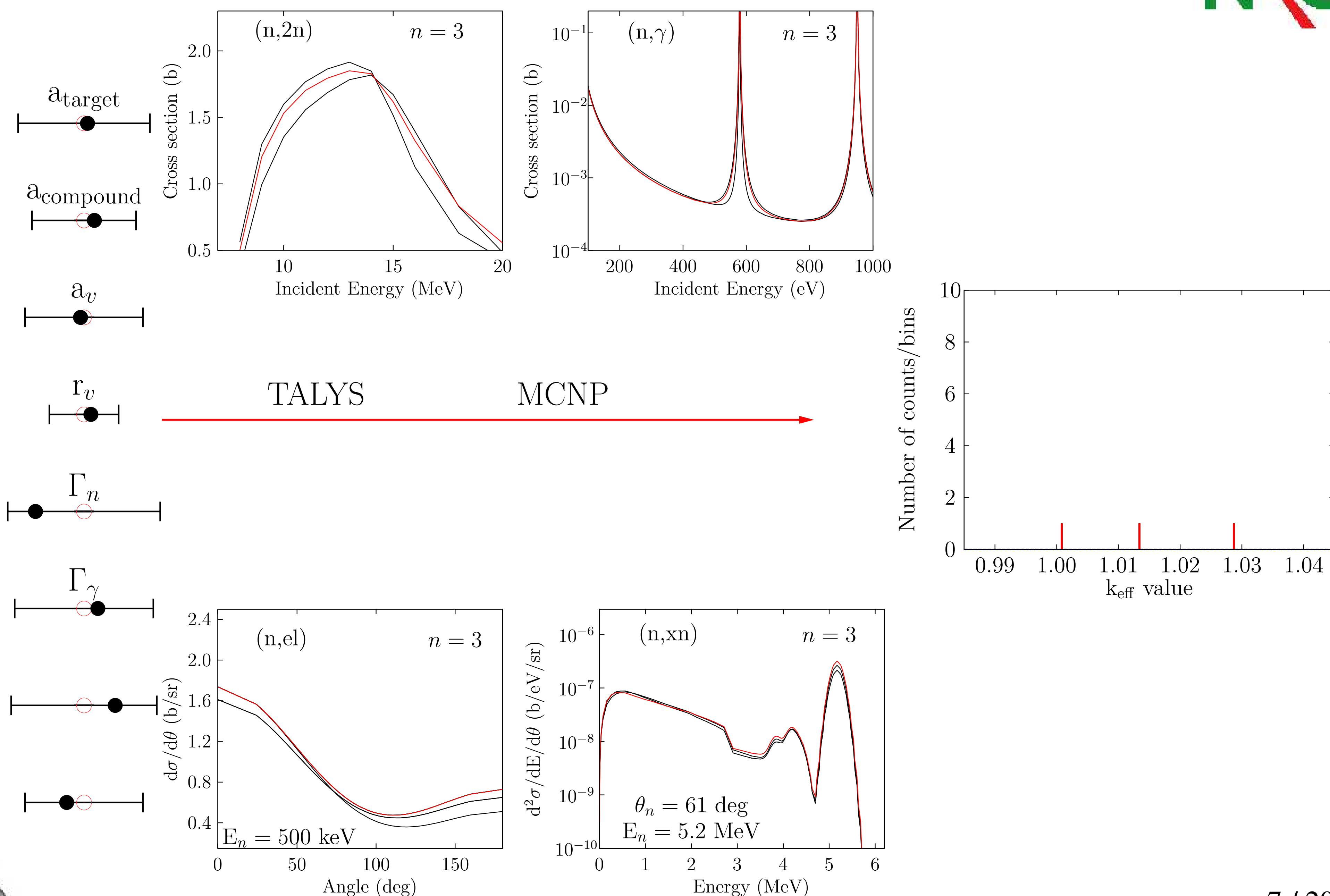

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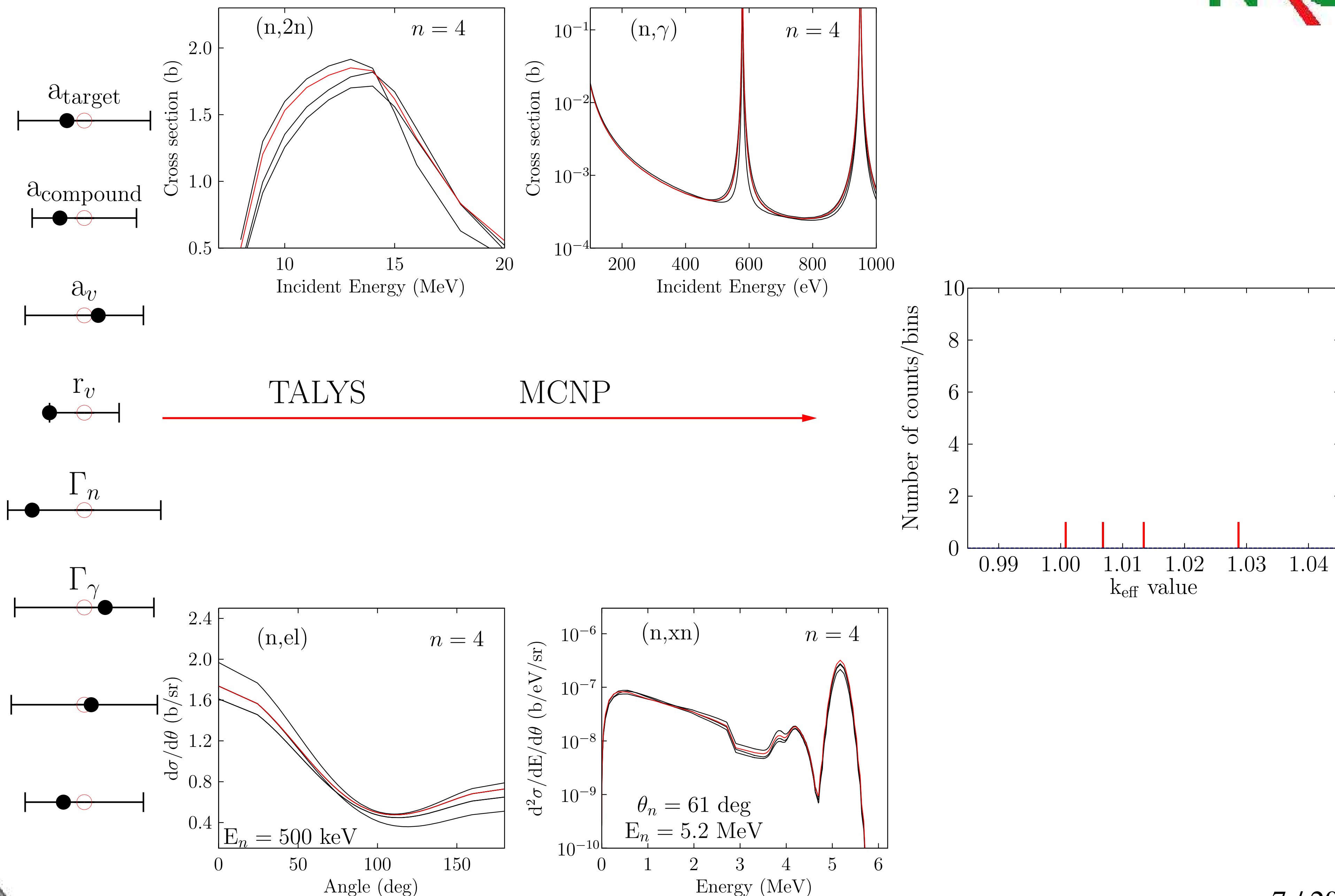

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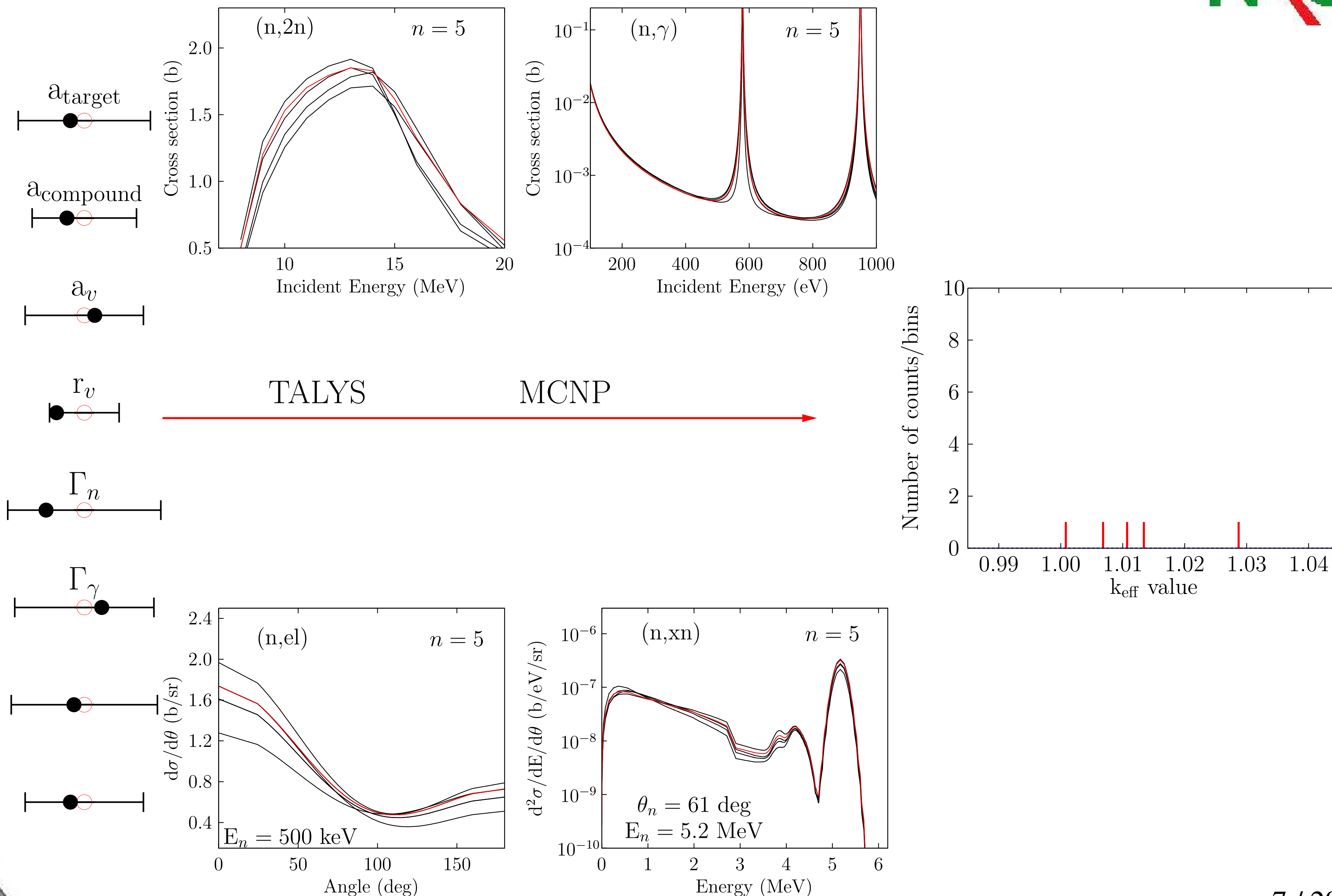

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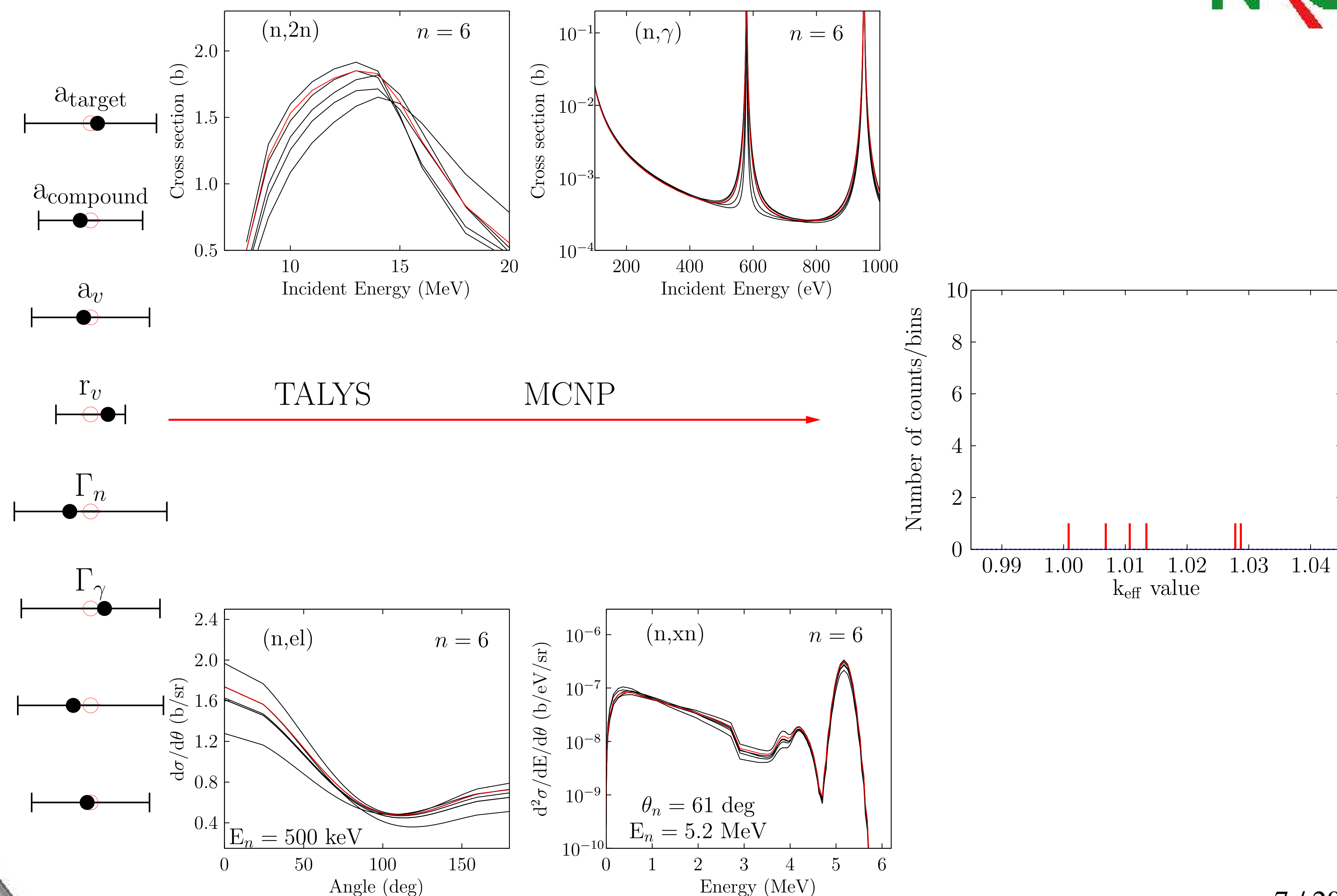

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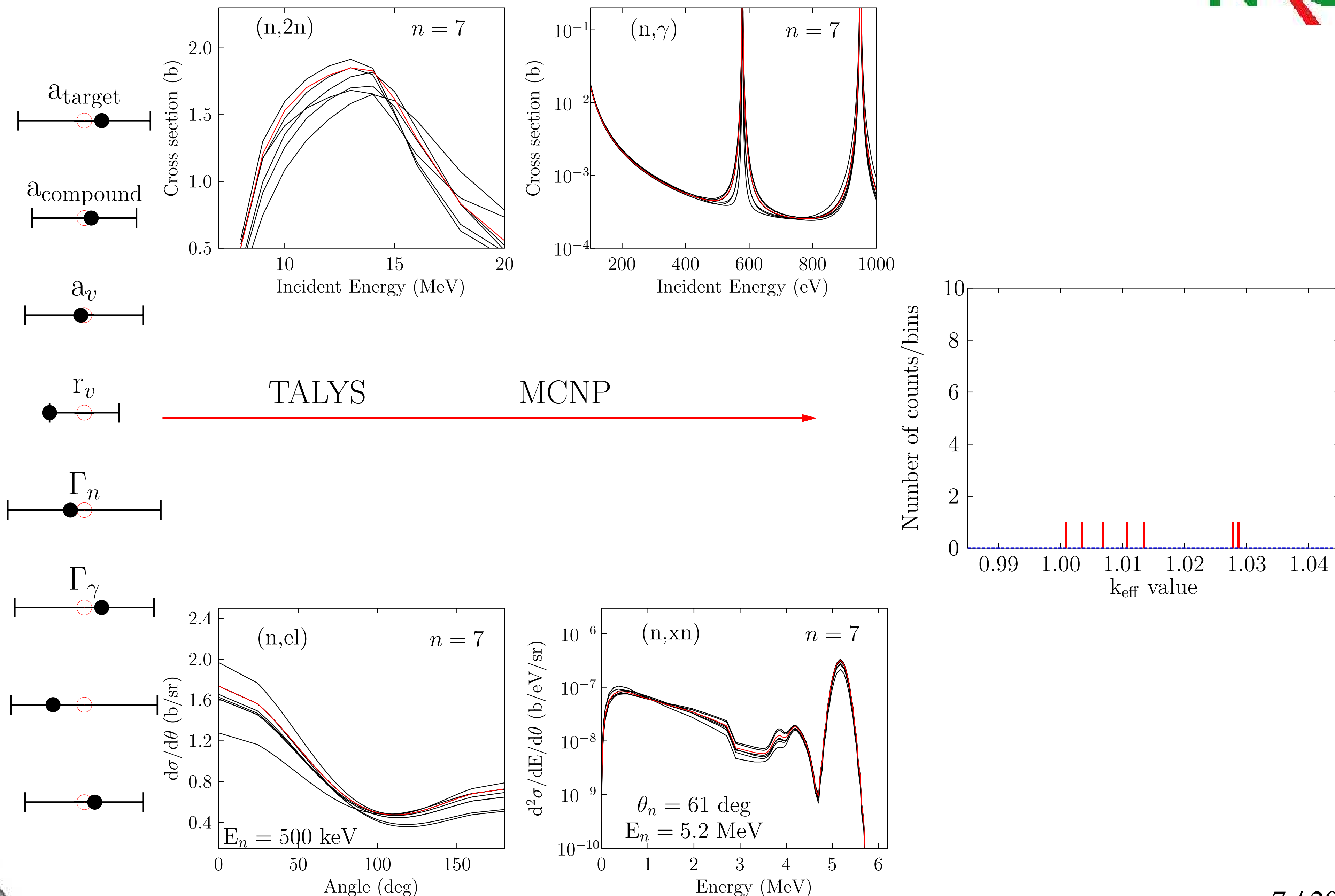

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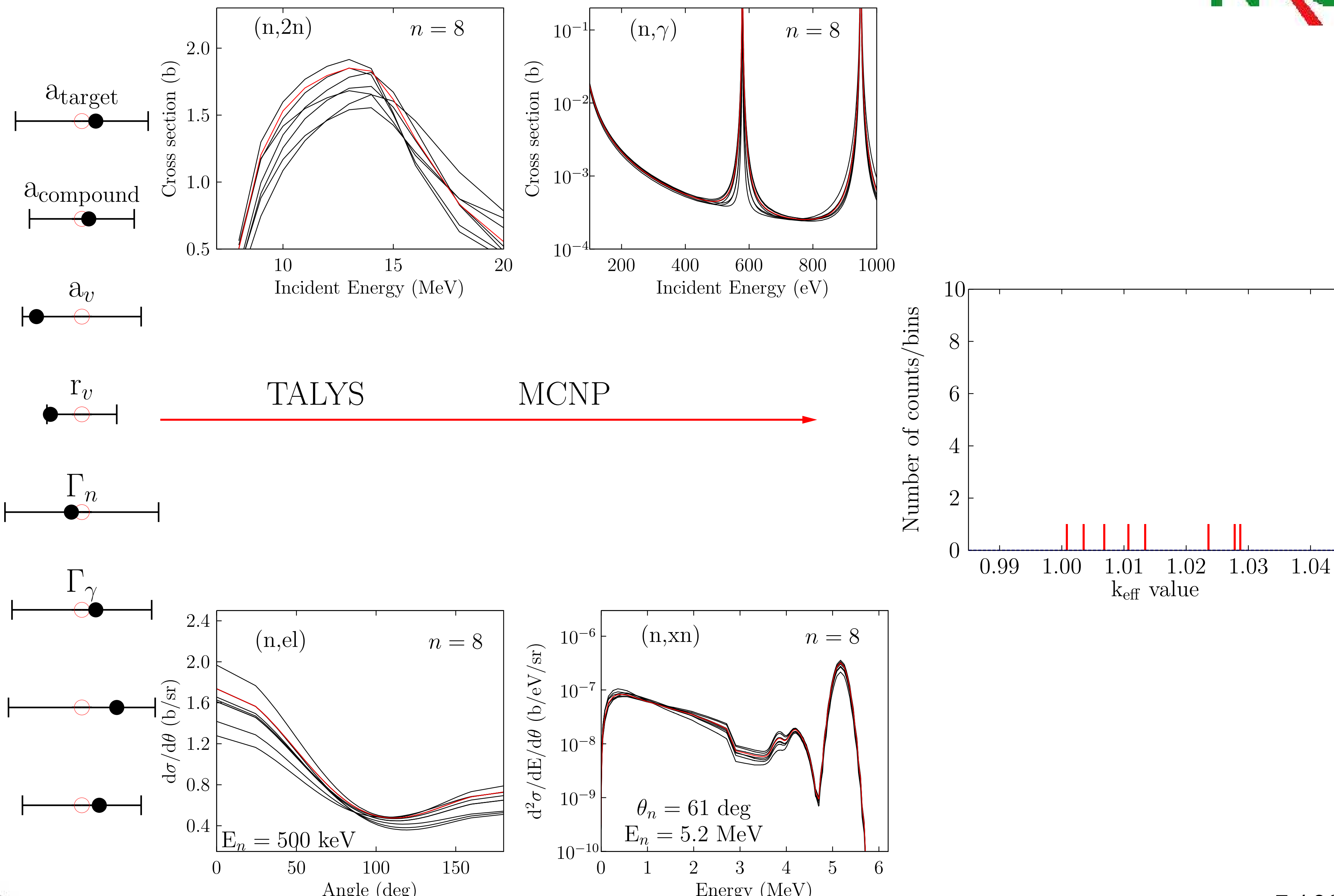

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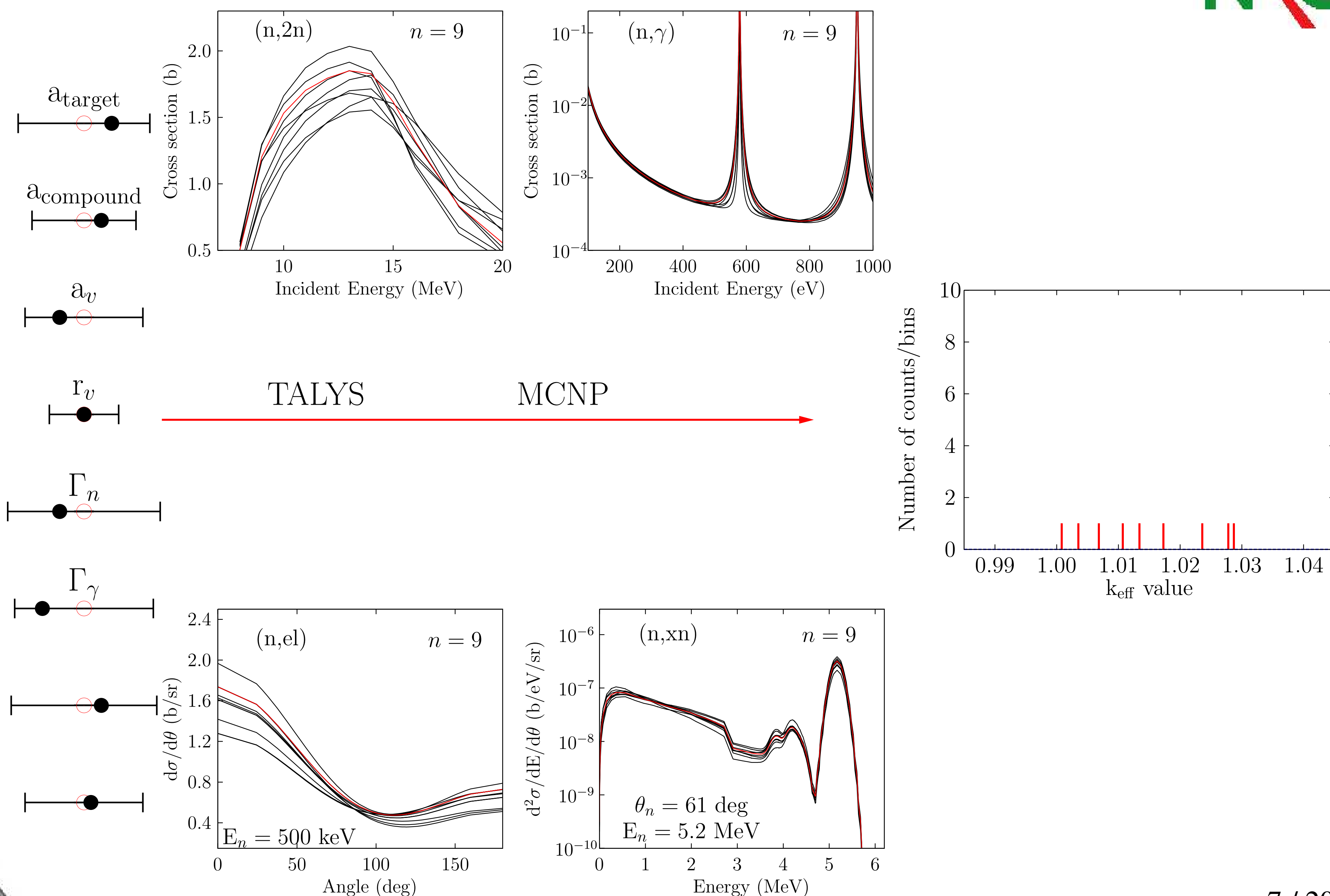

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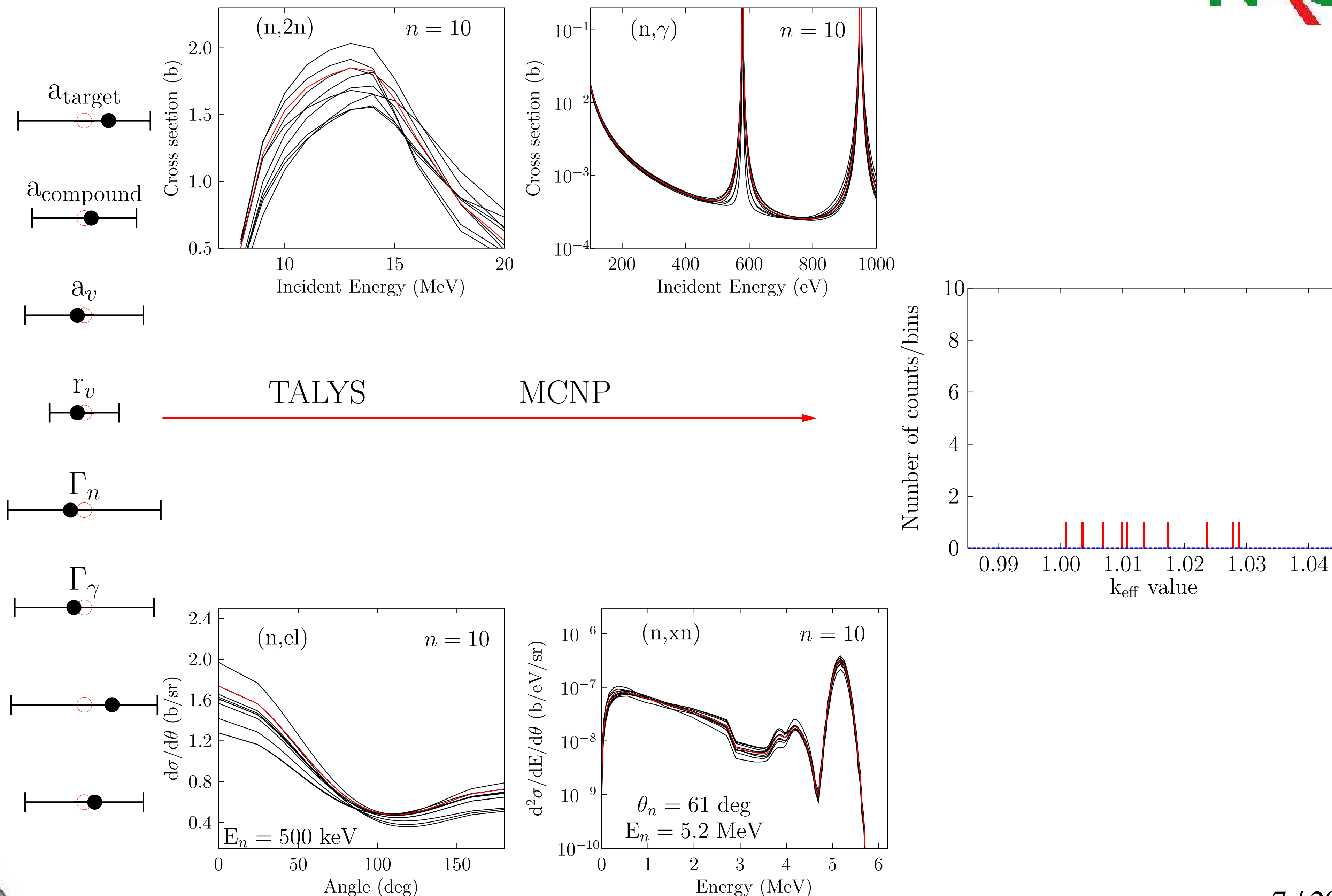

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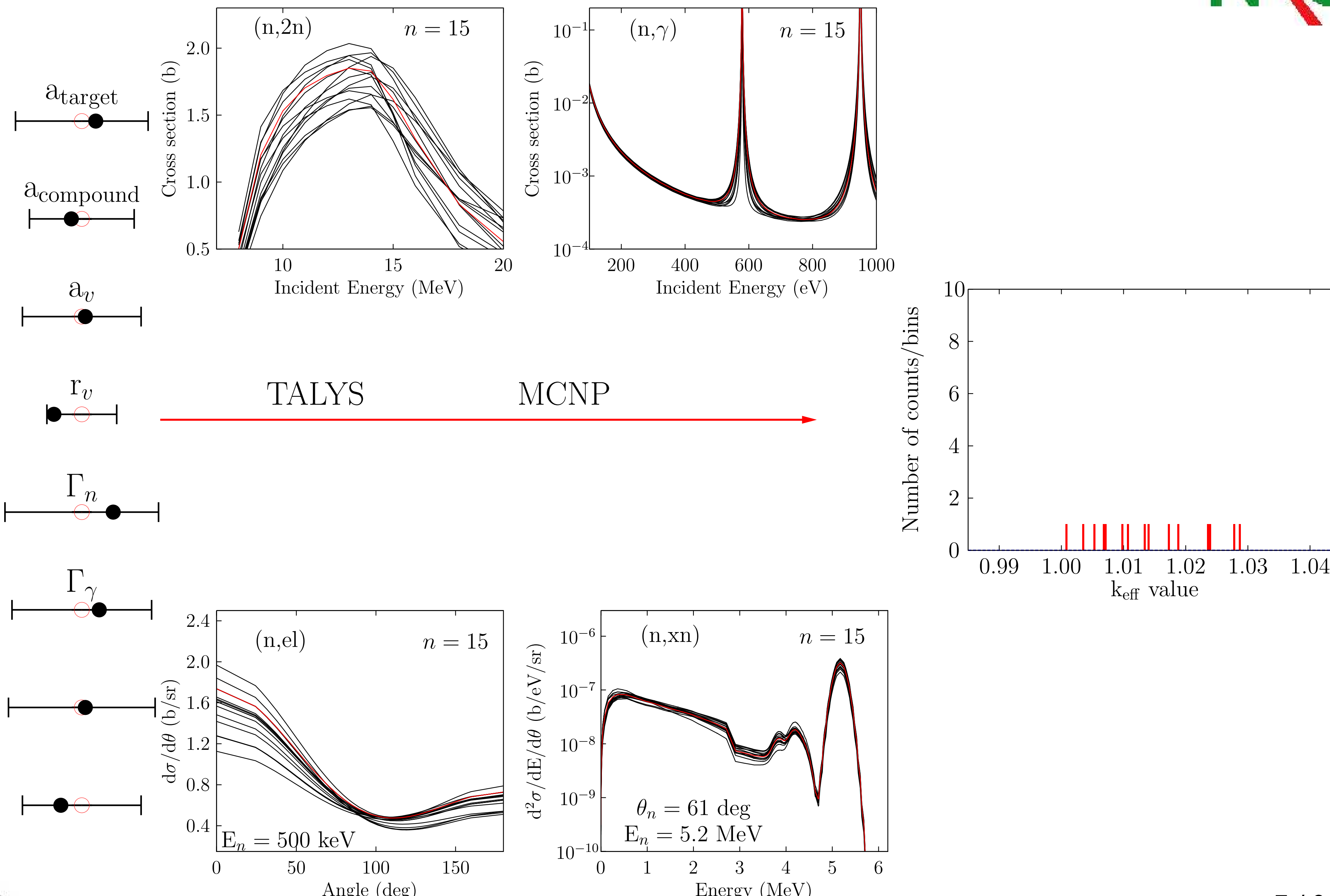

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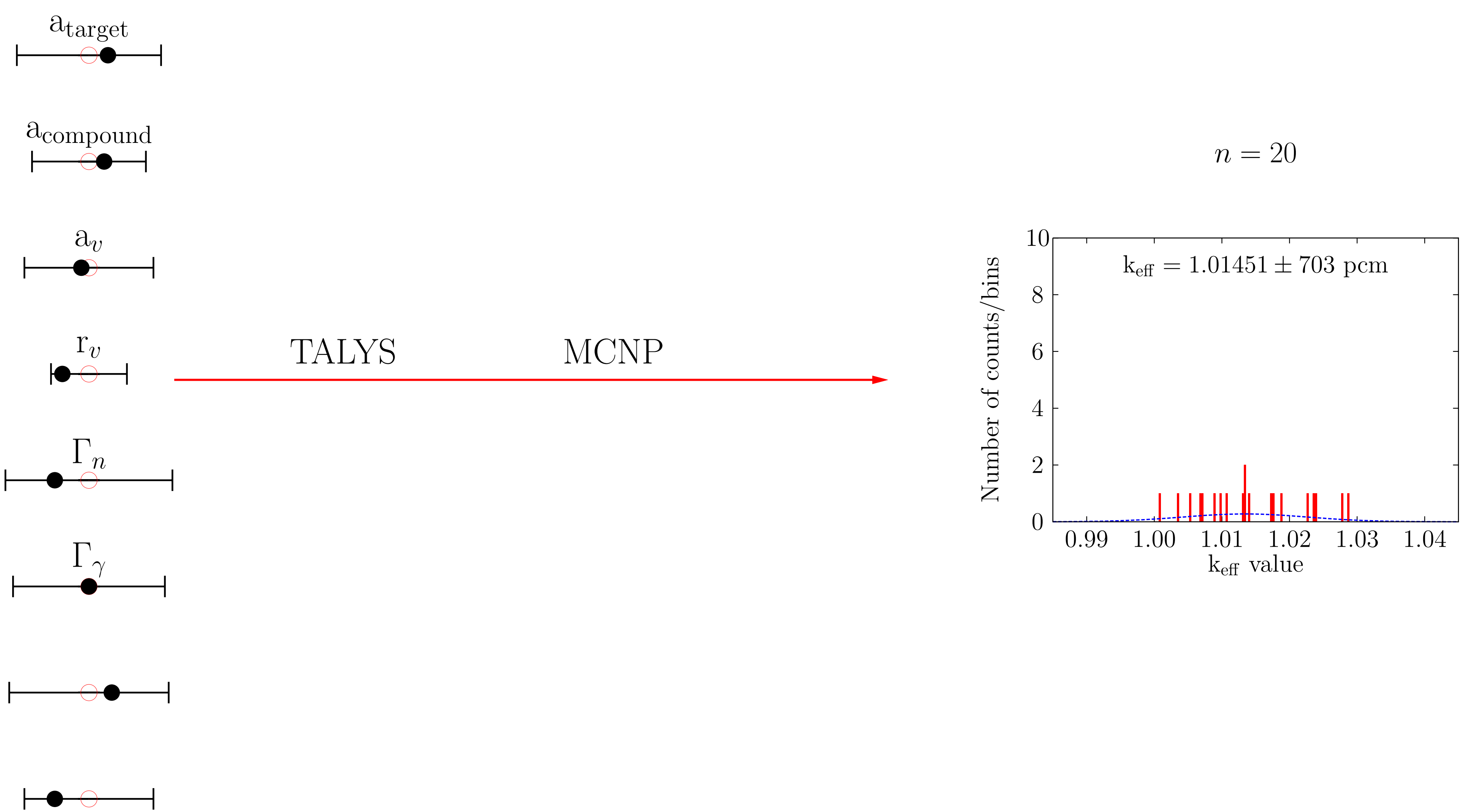

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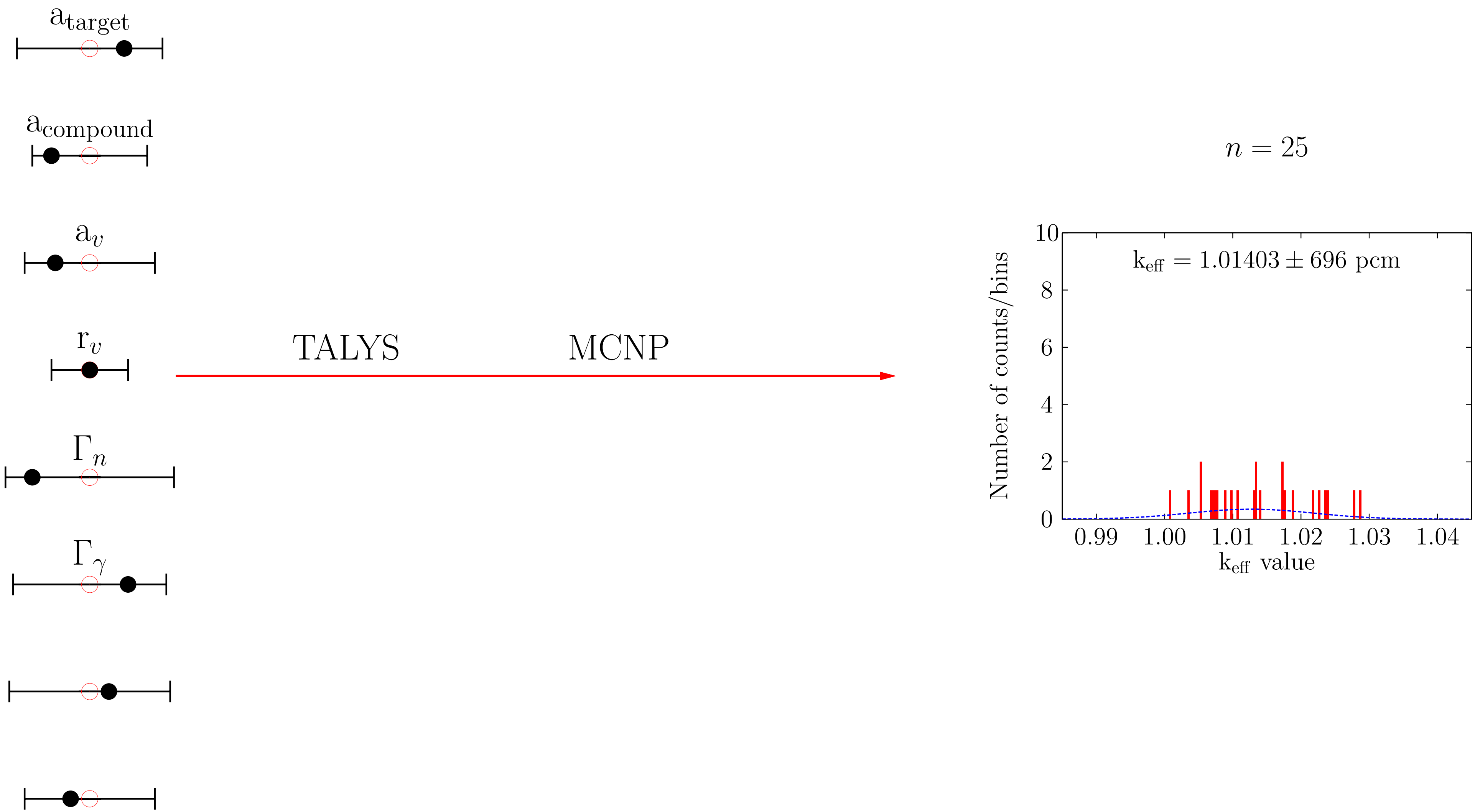

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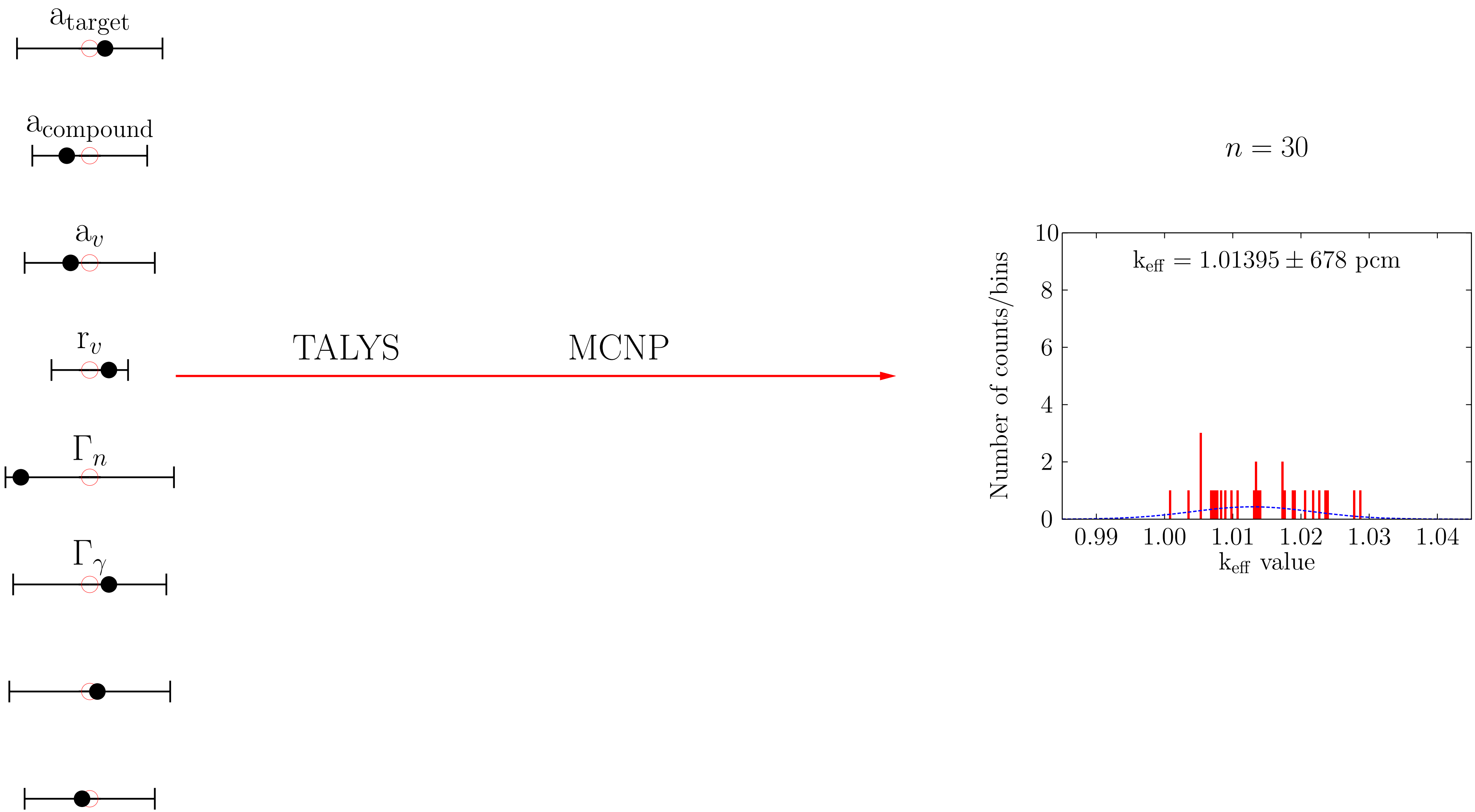

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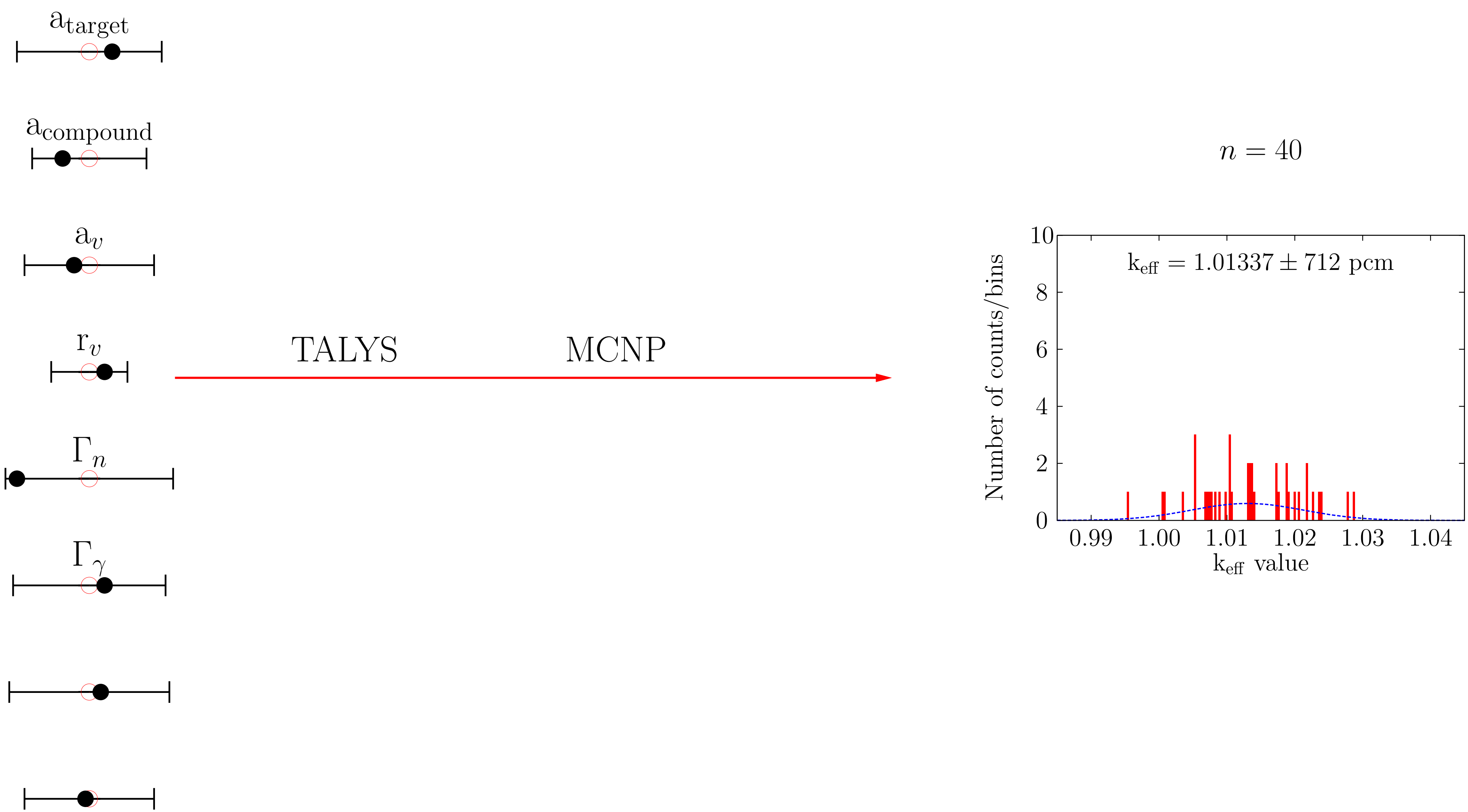

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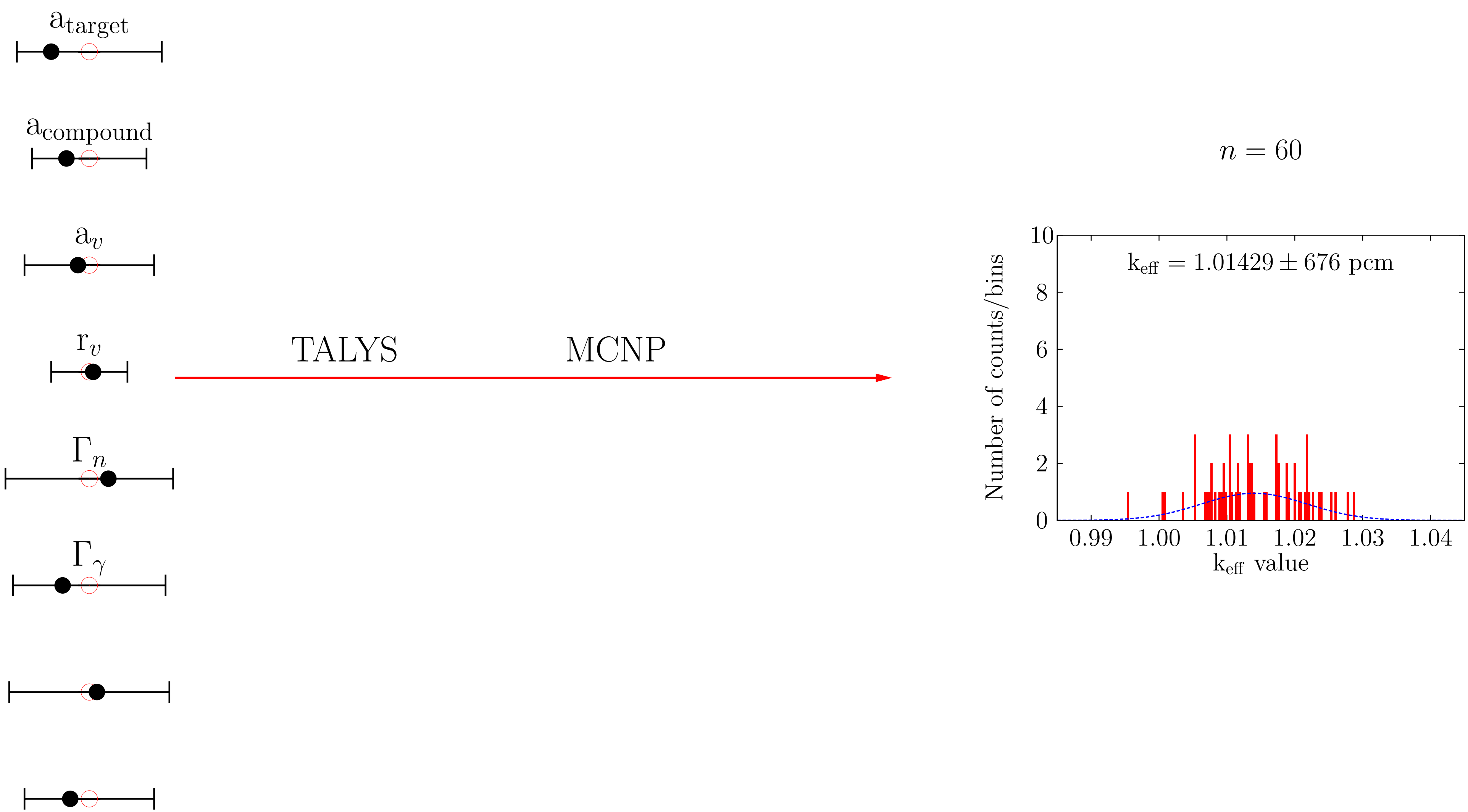

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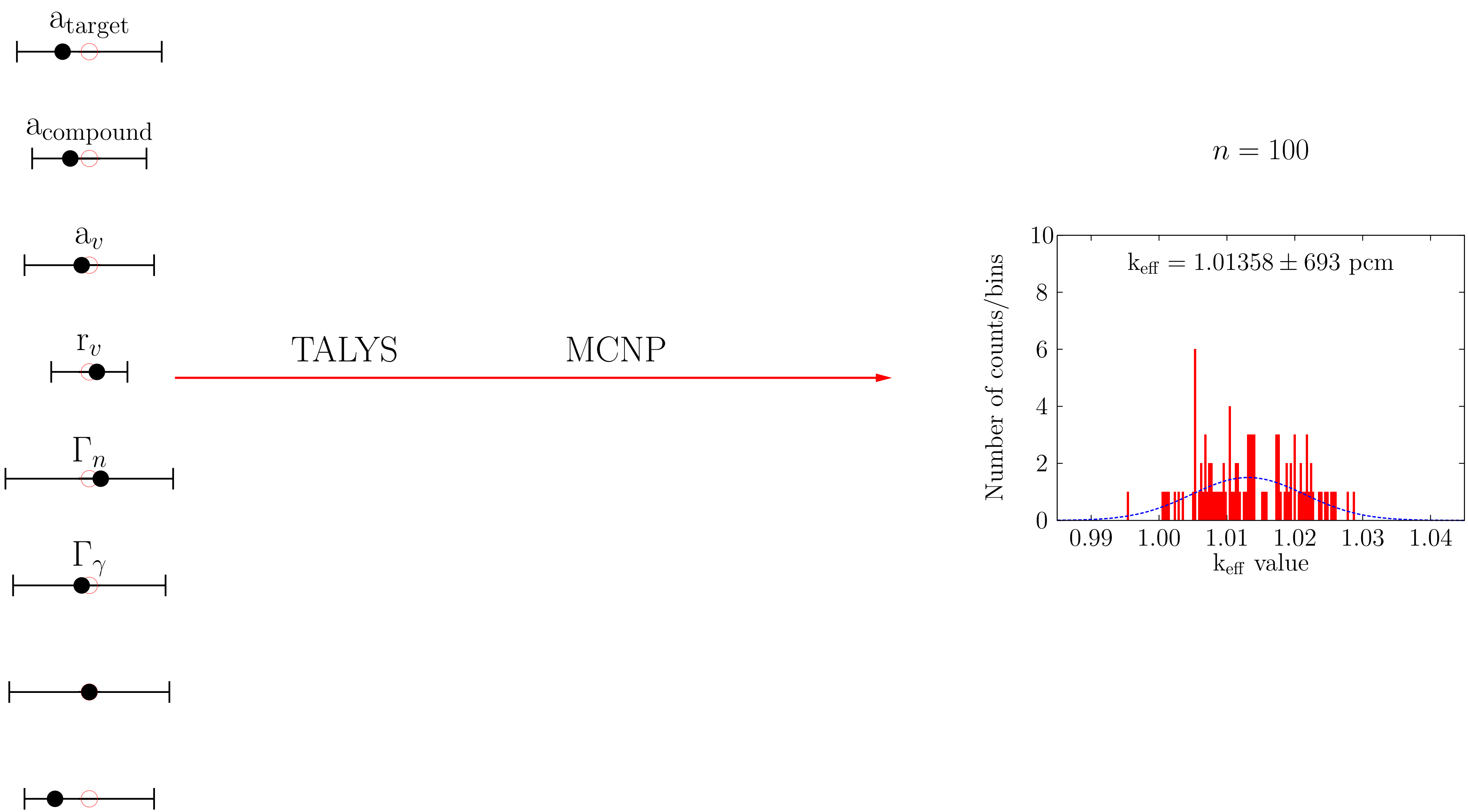

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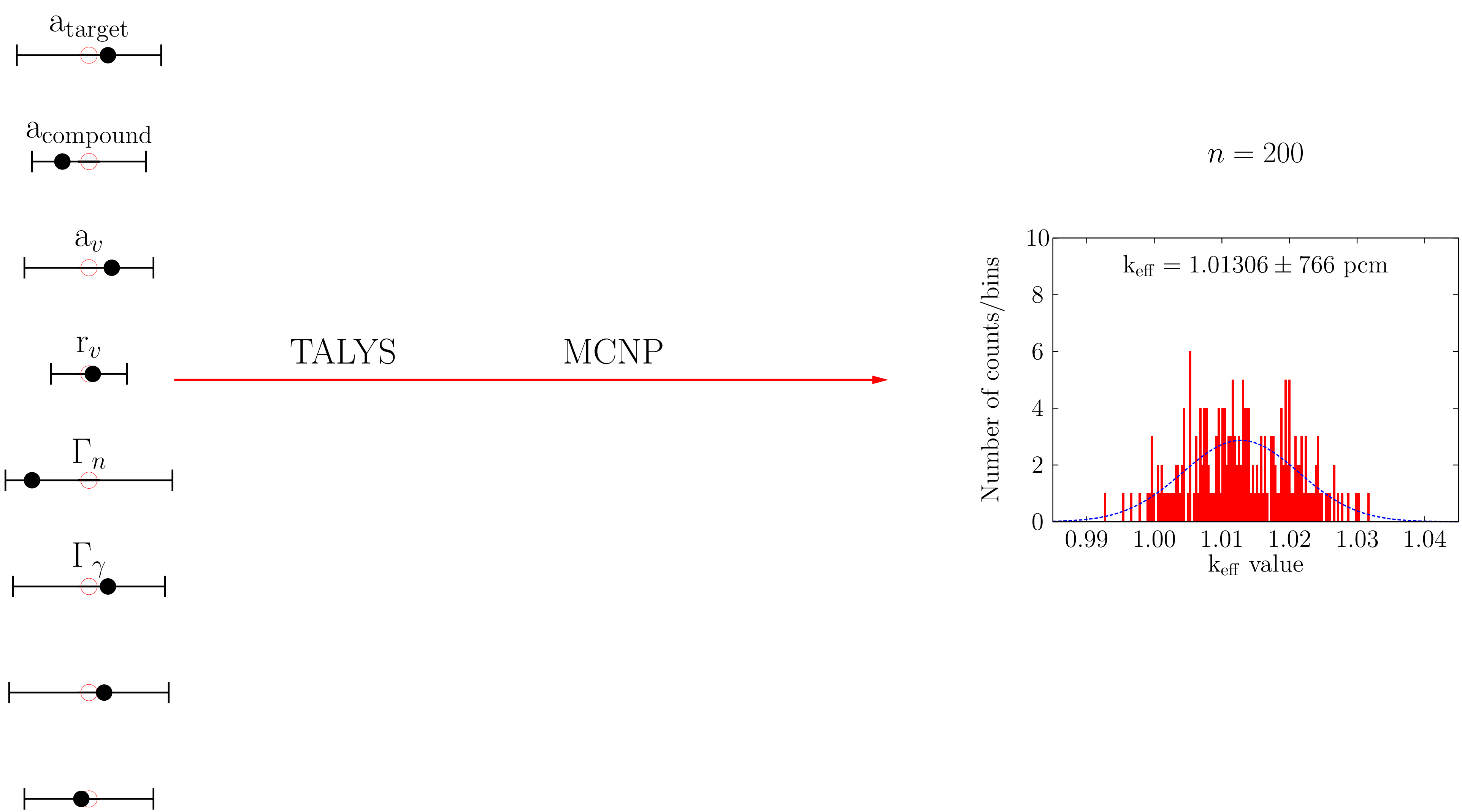

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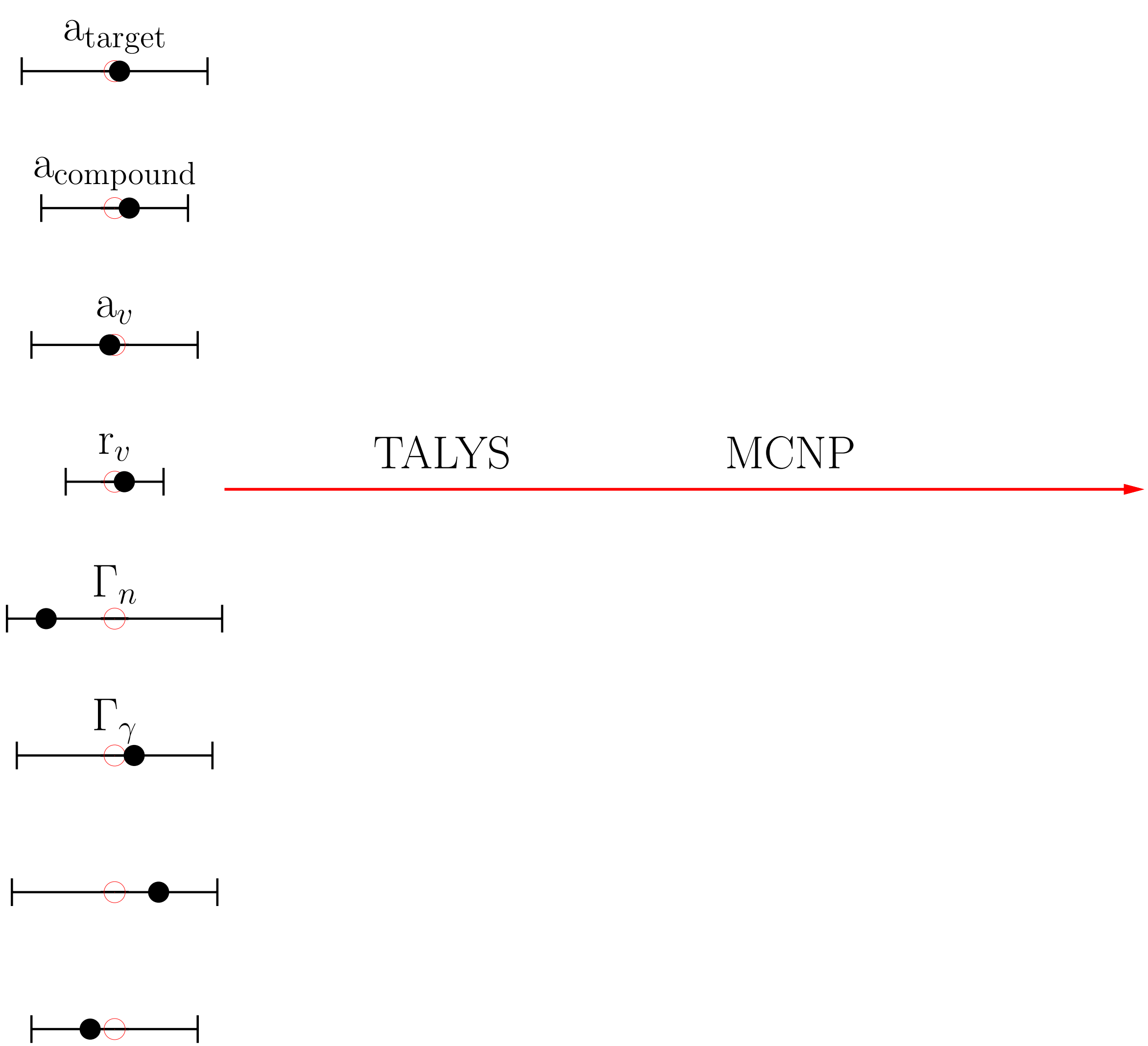
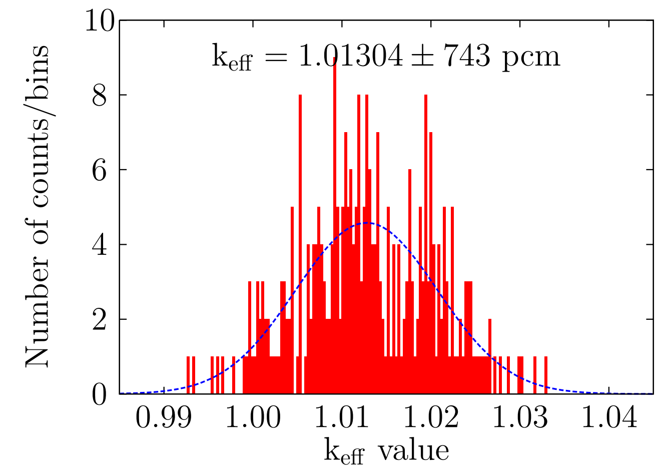


$n = 300$



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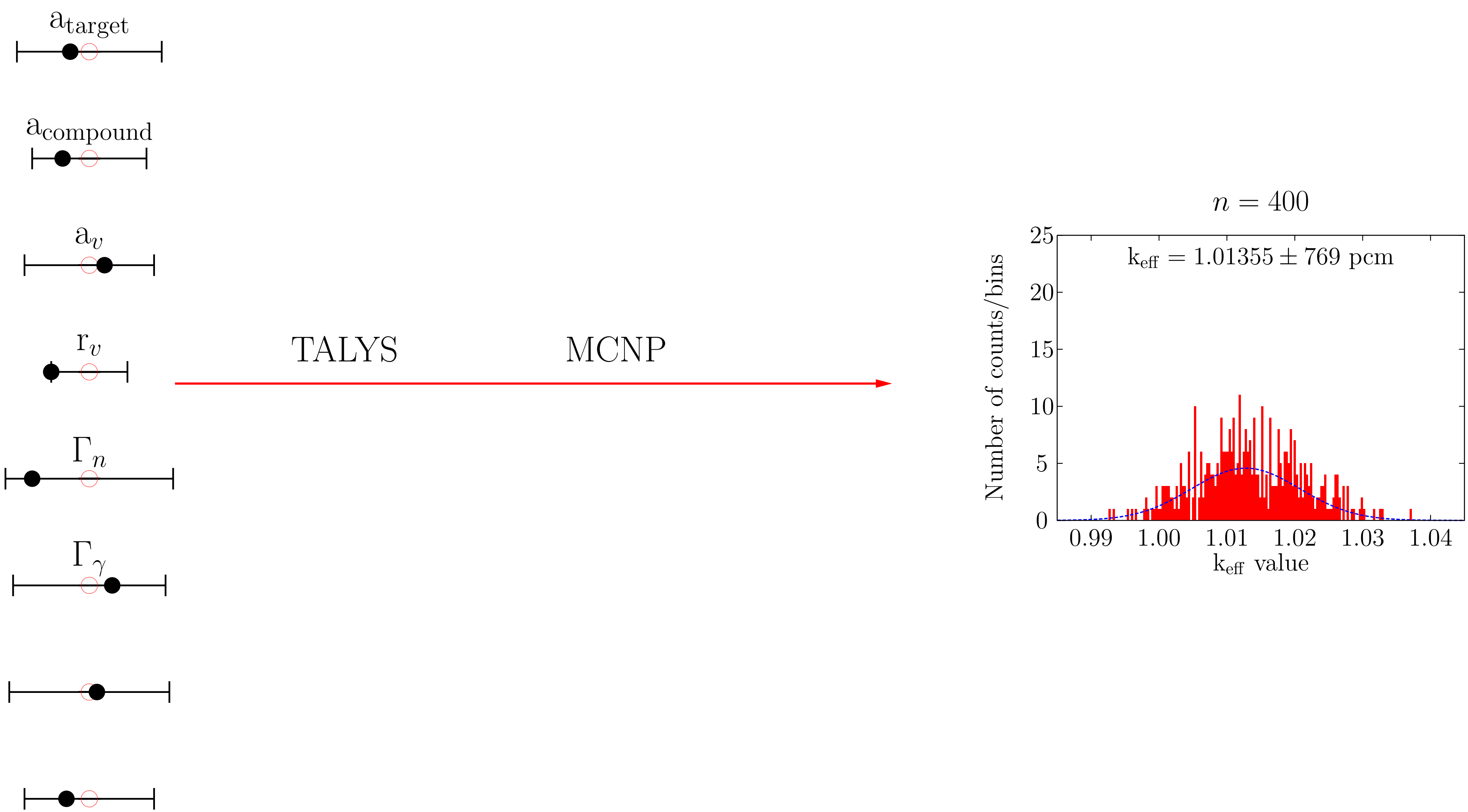

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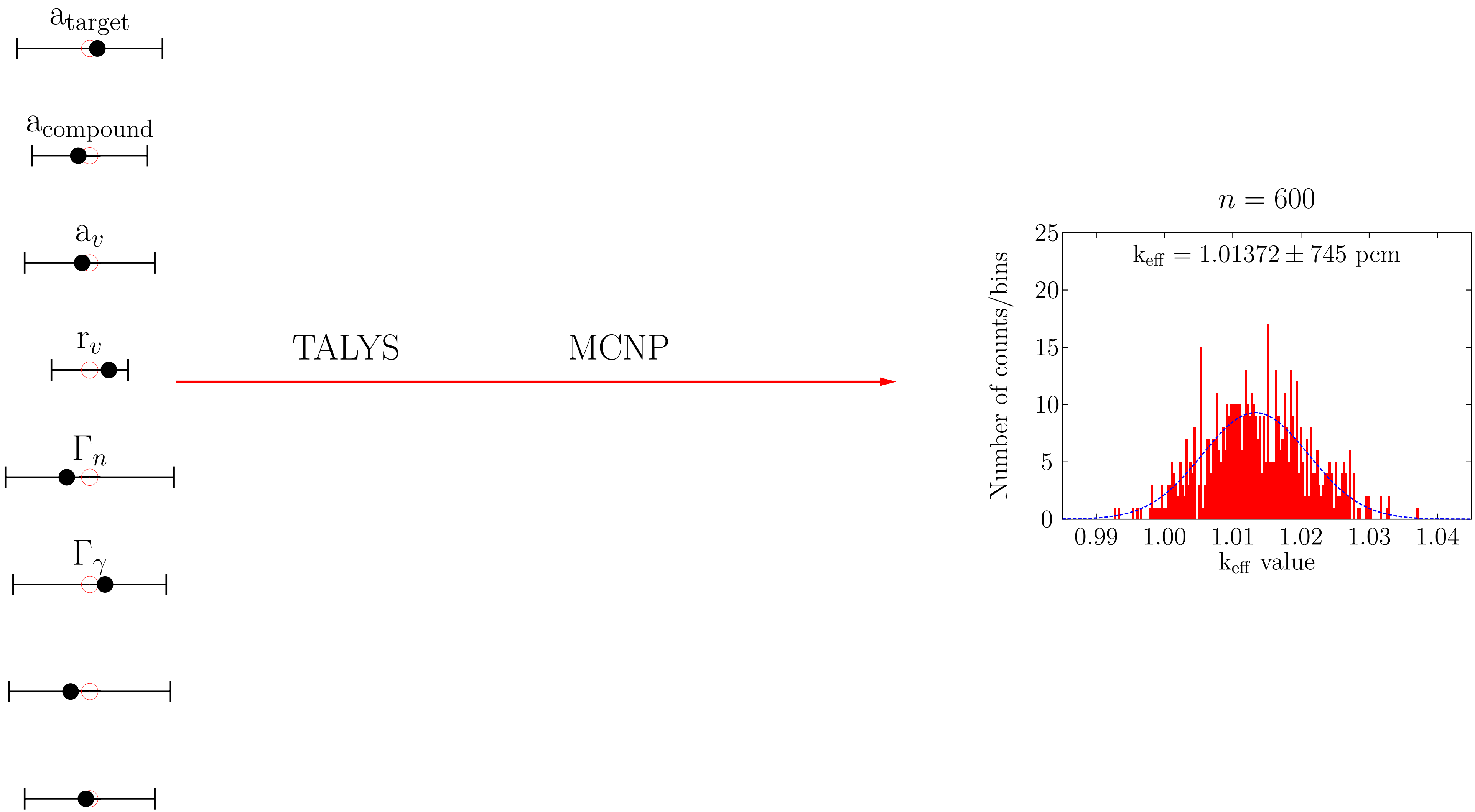

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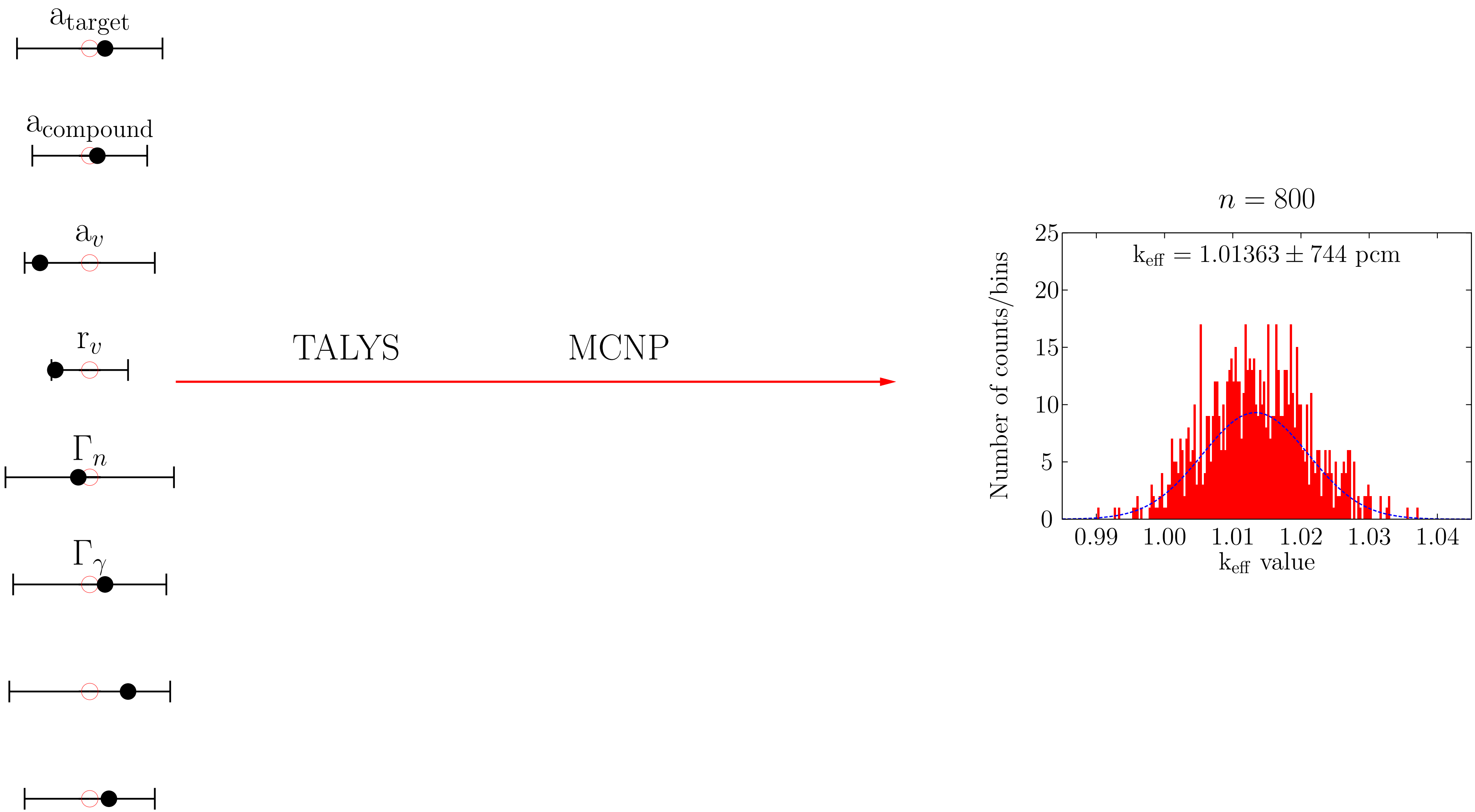

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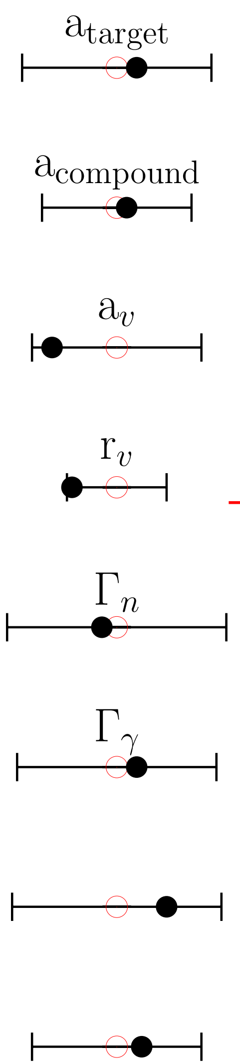

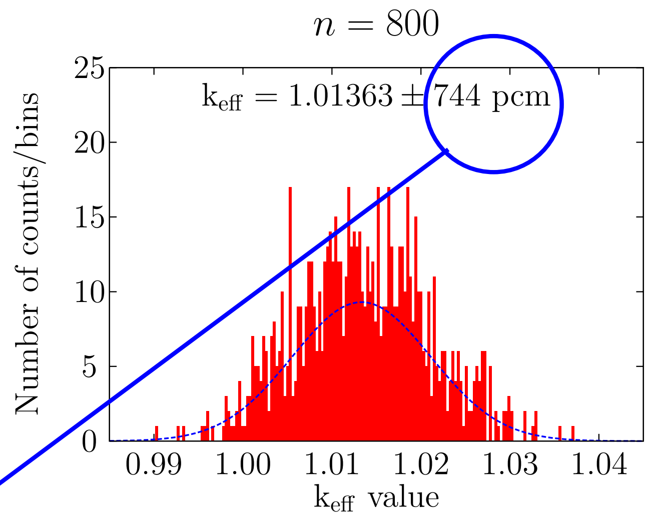

Statistical uncertainty $\simeq$ 68 pcm

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

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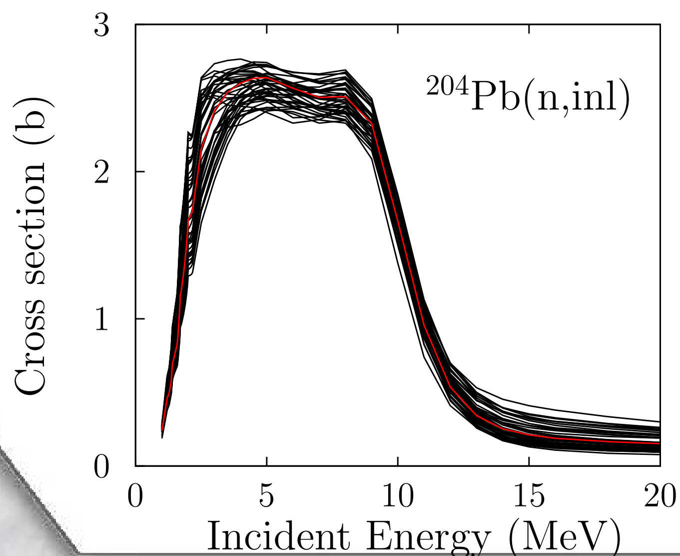
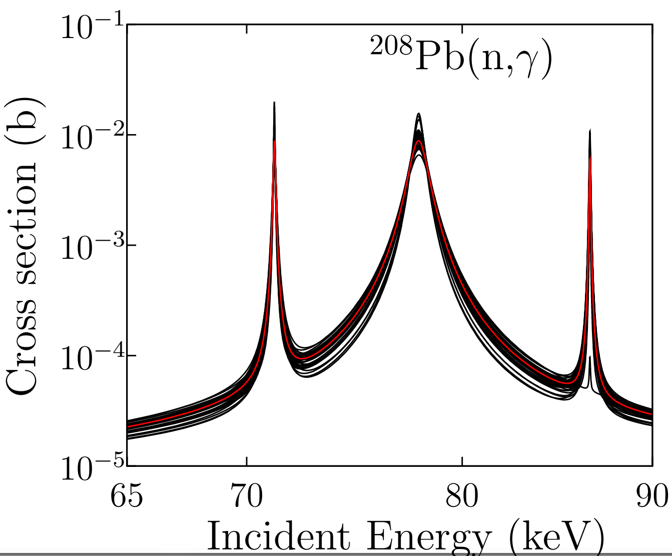
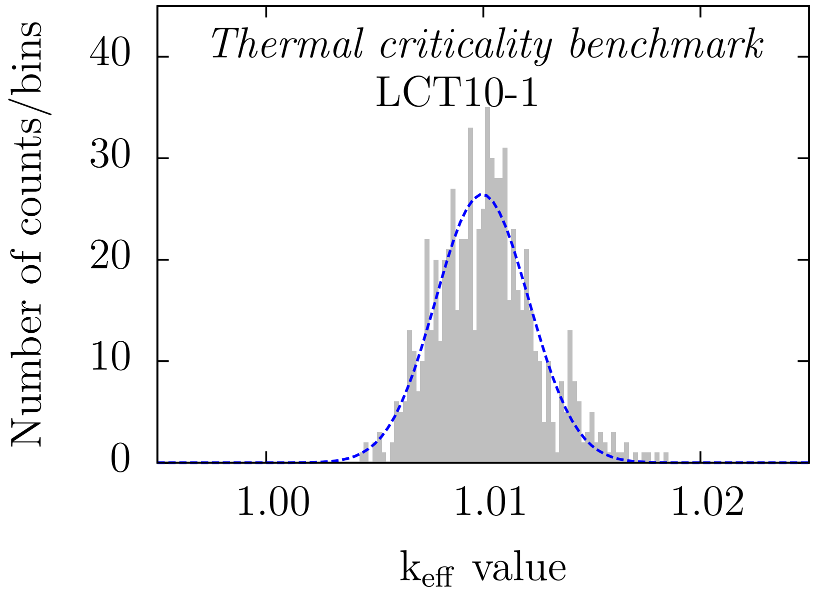
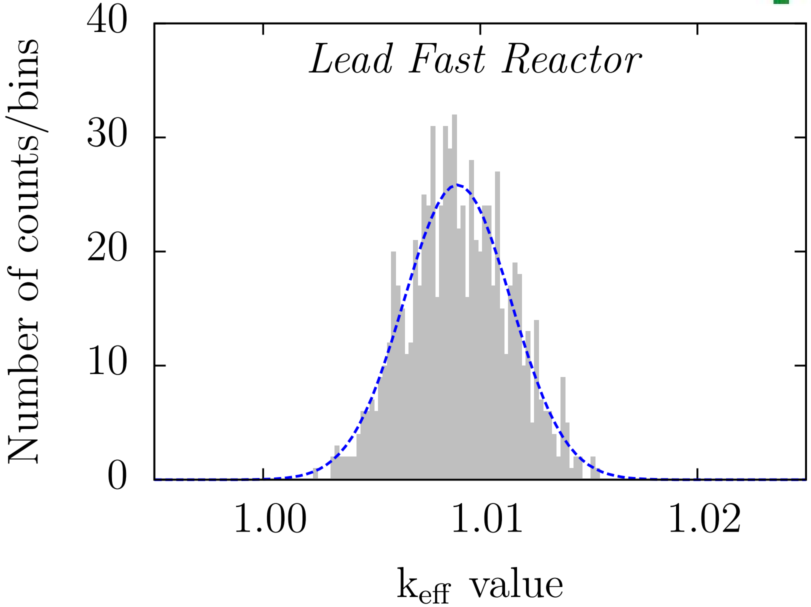
- $^{204-208}$Pb evaluations (NIM A589 (2008) 85) + **5000** random ENDF files
- Applied on k_{eff} and β_{eff} for criticality benchmarks (LCT-10 and HMF-64) and to ADS and LFR



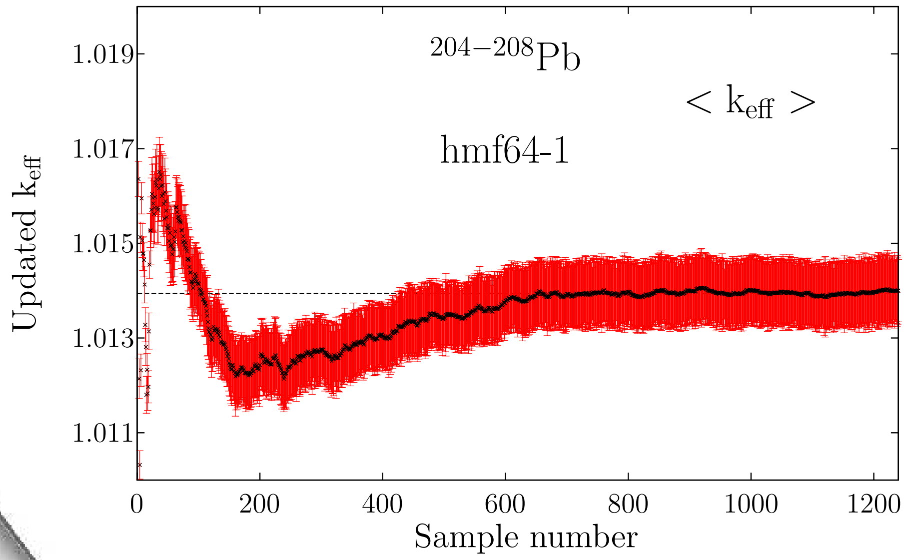


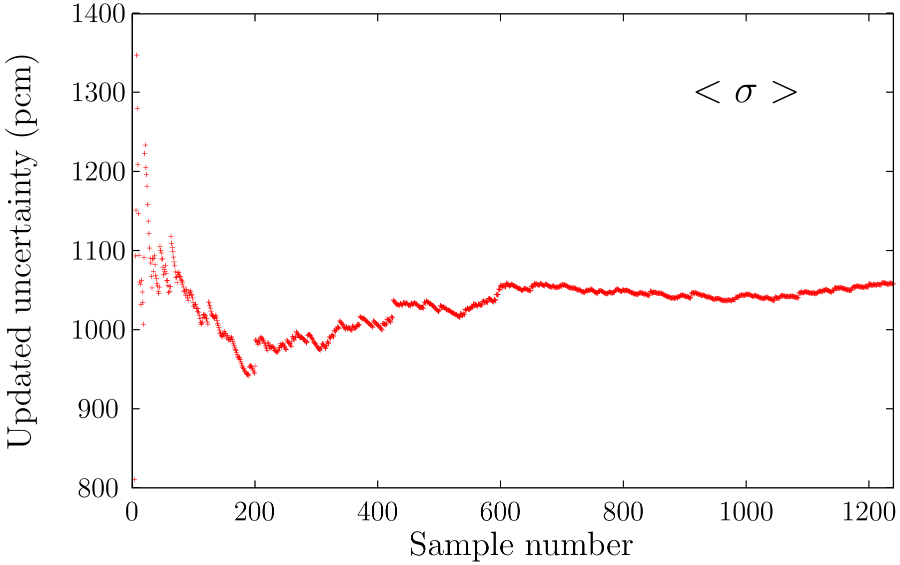
Examples with Pb isotopes



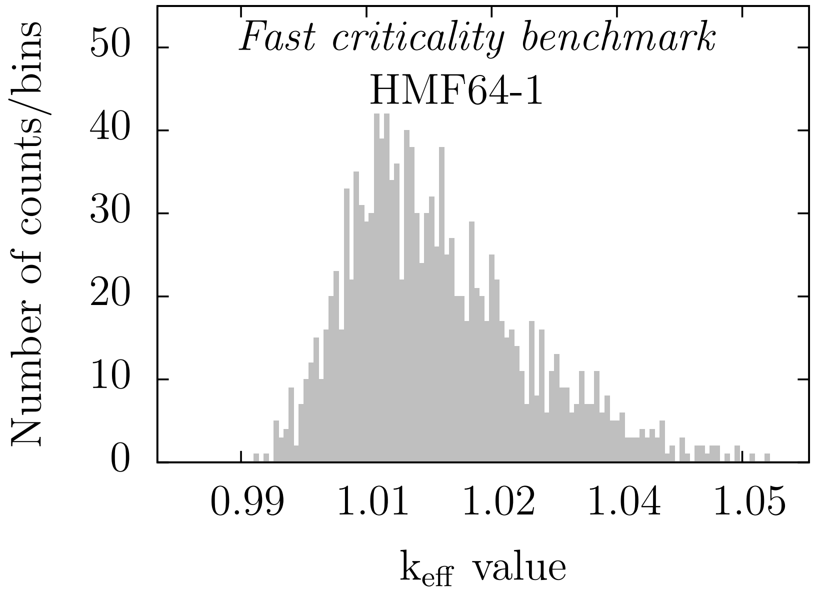


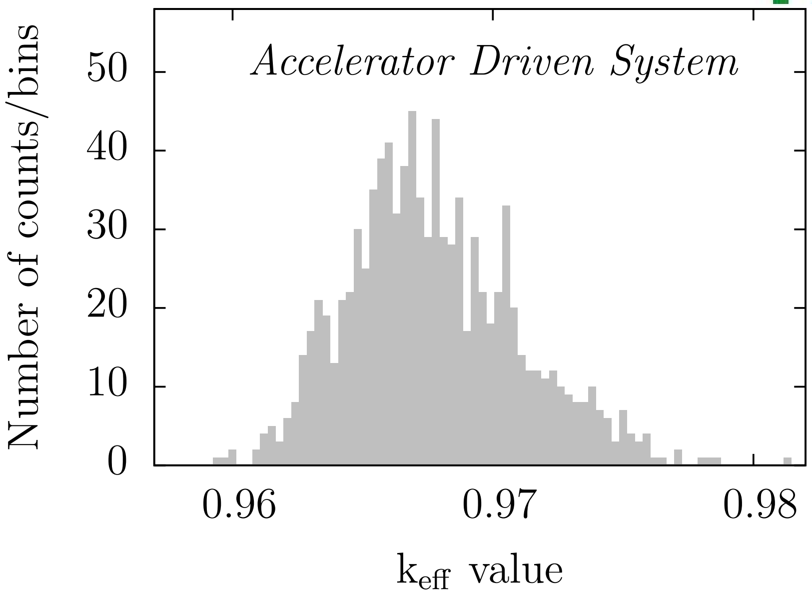
$k_{eff} = 1.01028 \pm (60 \text{ pcm and } 212 \text{ pcm})$ $k_{eff} = 1.00894 \pm (60 \text{ pcm and } 240 \text{ pcm})$





Examples with Pb isotopes





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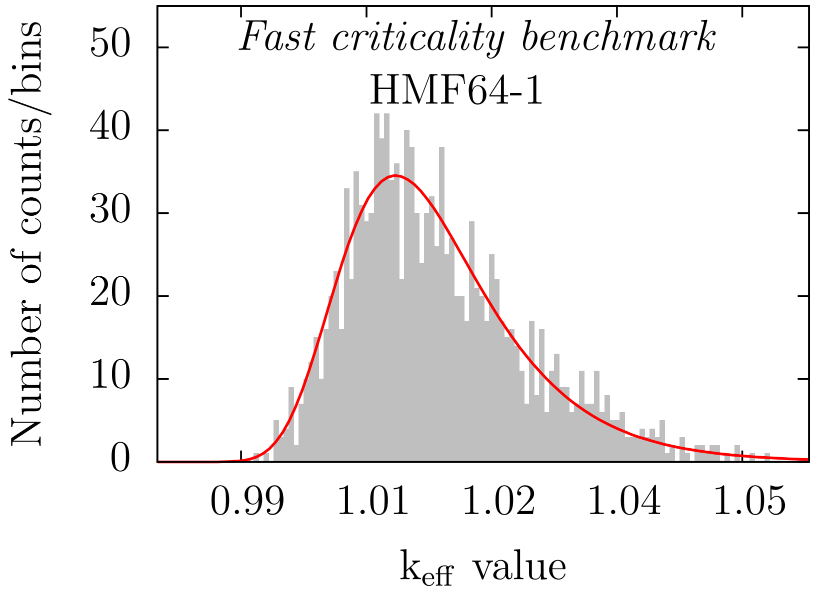
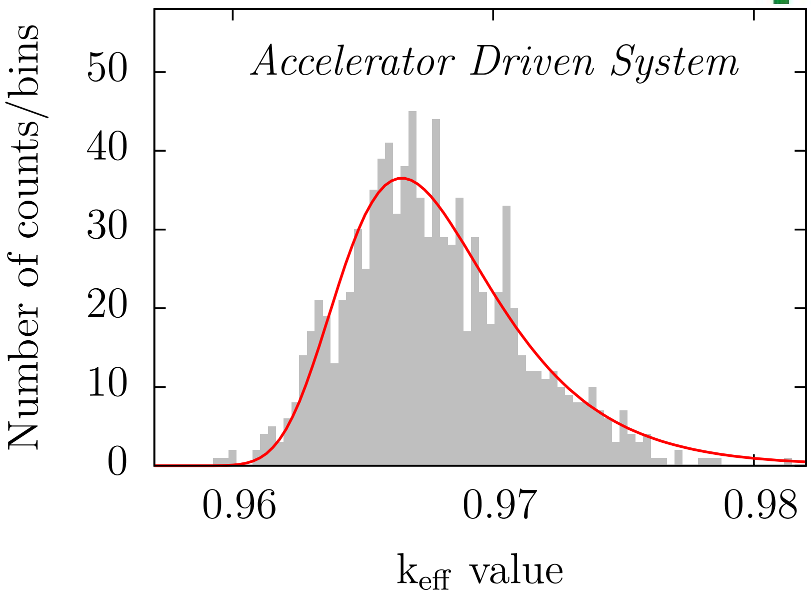




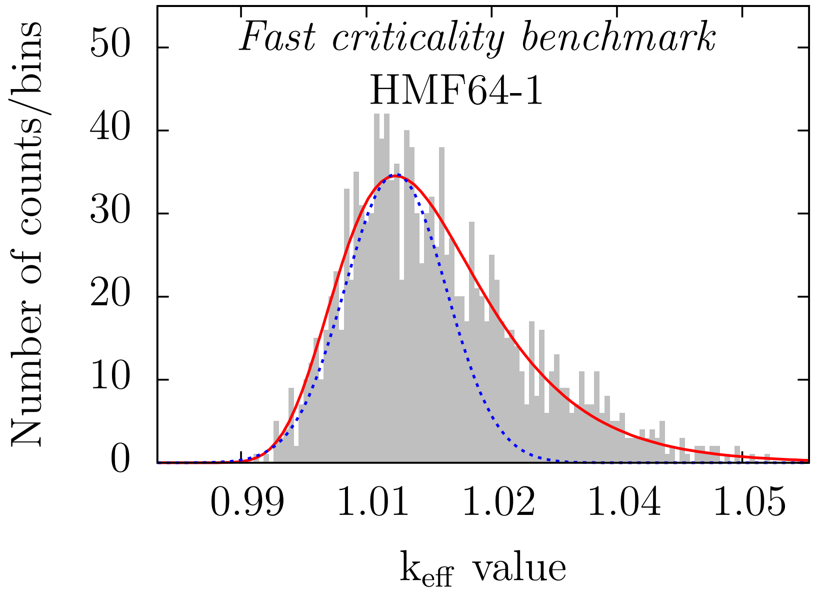
Better fit with the "*Extreme Value Theory*", or EVT:

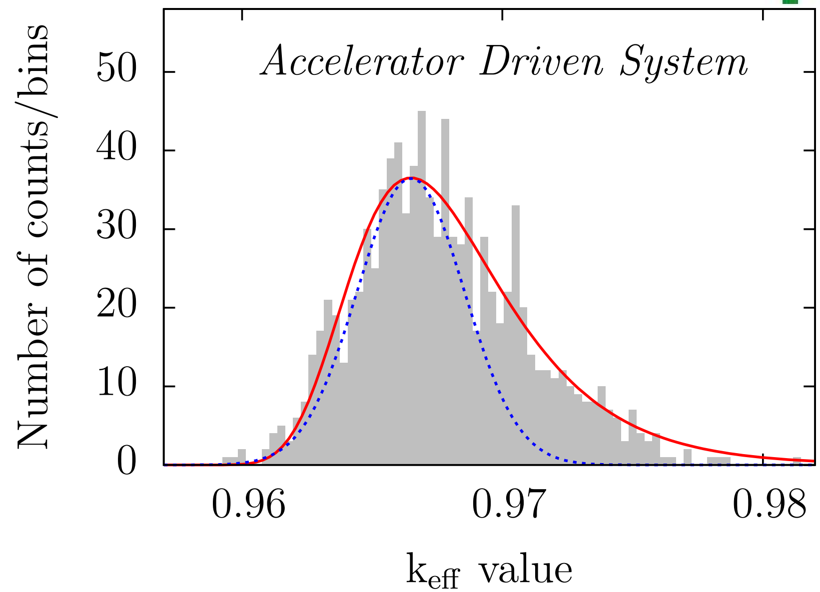
$F(z) = e^{-z-e^{-z}}$ with $z = \frac{X-\mu}{\sigma}$

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

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

Examples with Pb isotopes





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	HMF-64.1	ADS
k_{eff}	1.00848	0.96648
	μ'=1.01394	μ'=0.96785
$\sigma_k \times 10^5$	**855**	**291**
	σ'=1097	**σ'=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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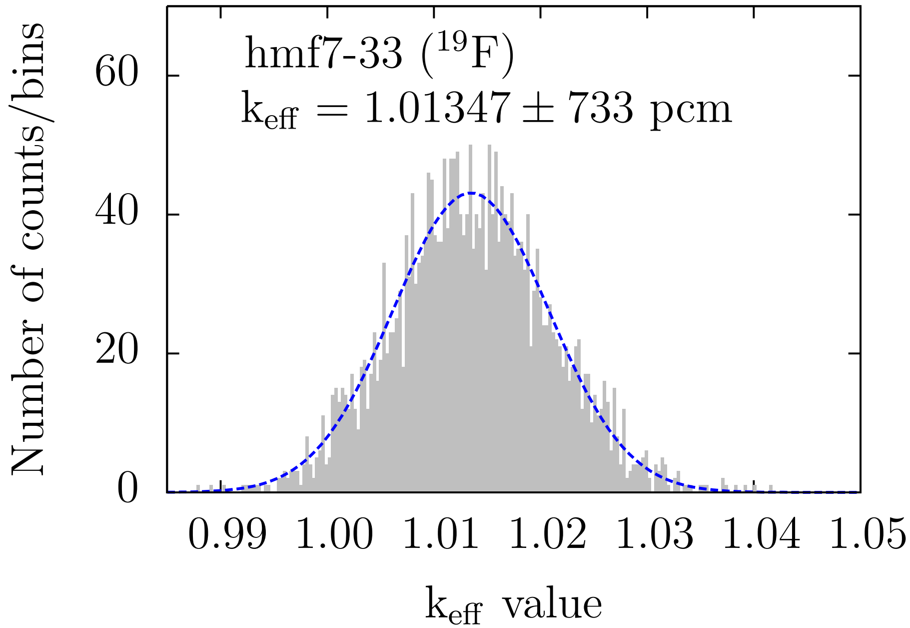
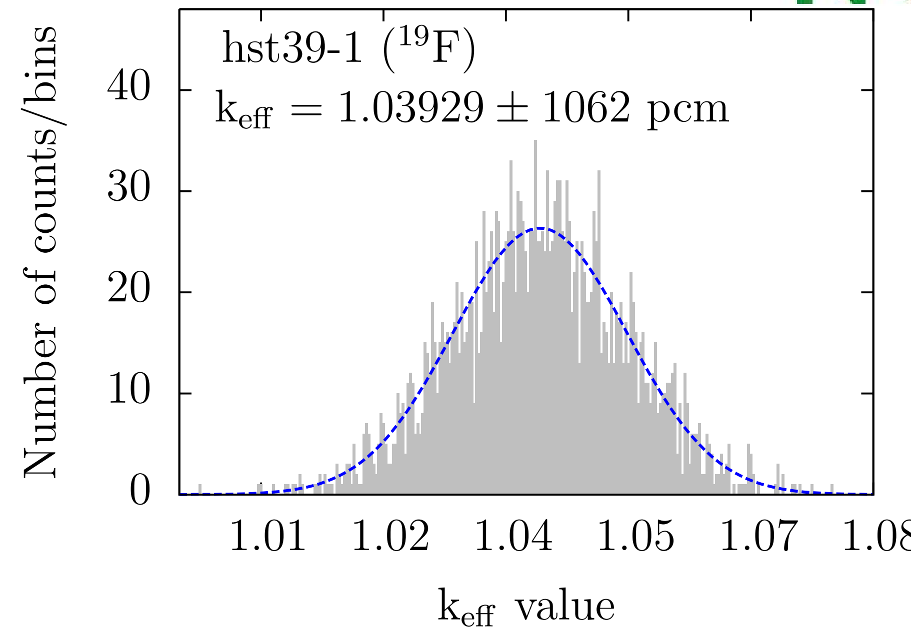
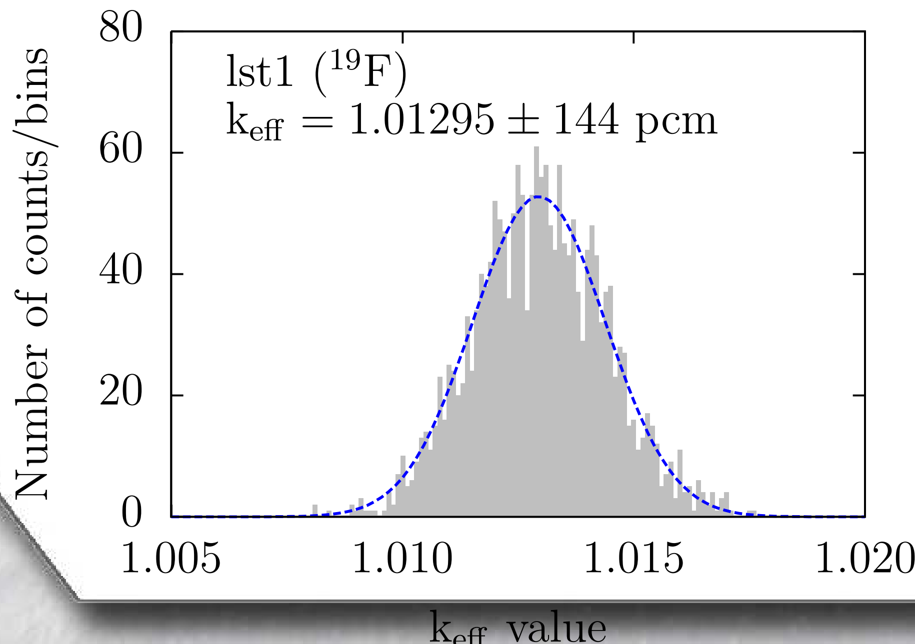
Okay, let's go from academic solutions (☕) to mass/applied production (🏭) !

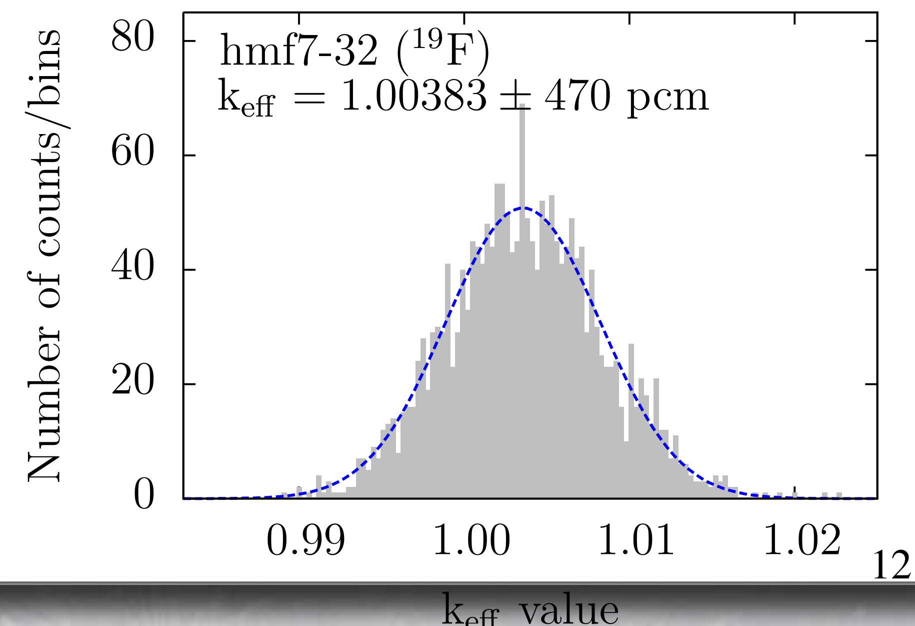
- Default TALYS calculation + Resonance parameters (RP) + uncertainties
- 100 to 2000 ENDF files per isotope from ^{12}C to ^{240}Pu ($\simeq$ 100 isotopes)
- 190 criticality-safety benchmarks ($>$ 60 000 calculations) from the ICSBP
- All Oktavian shielding benchmarks (neutrons and gammas)
- Reactivity 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

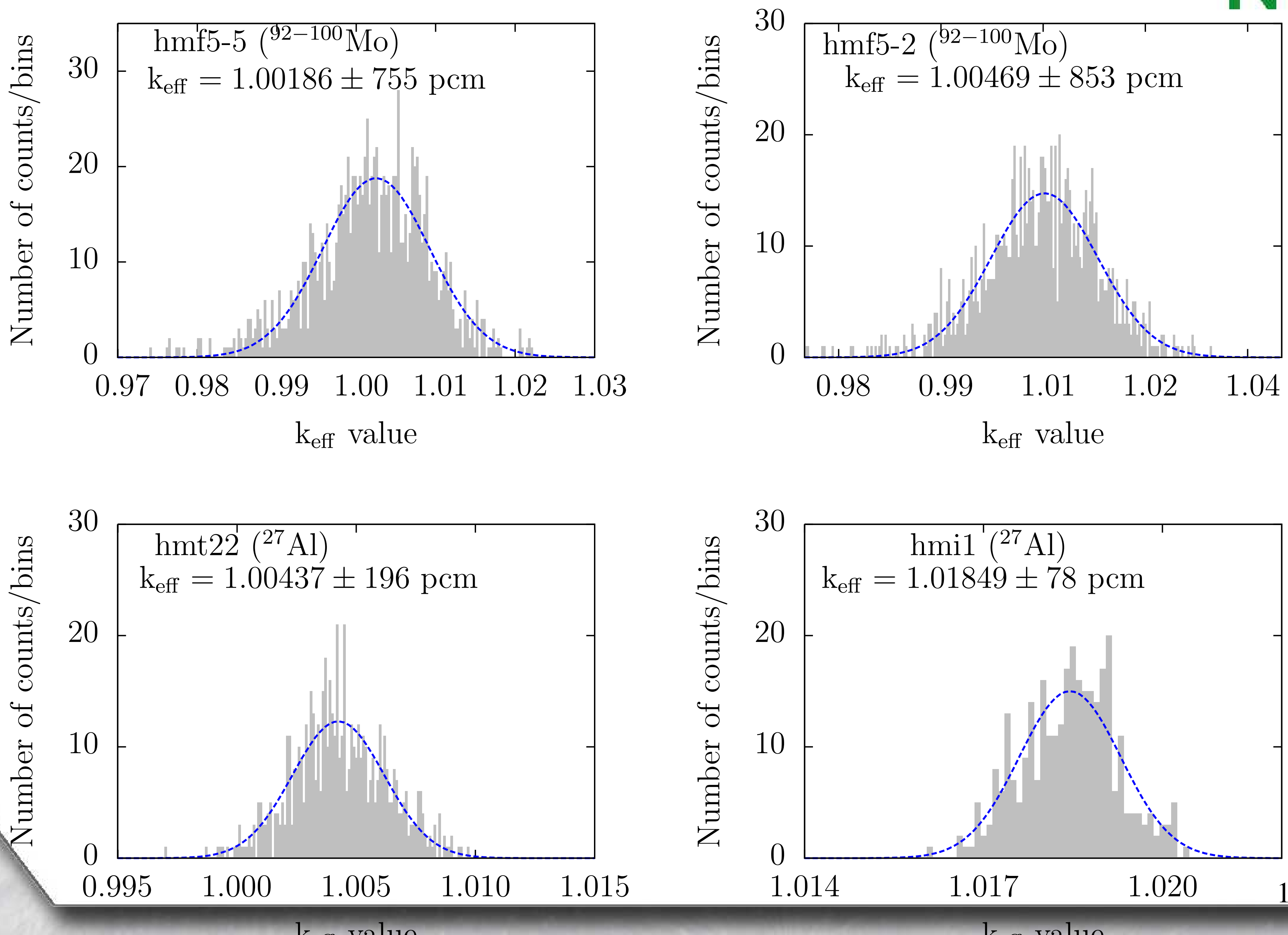




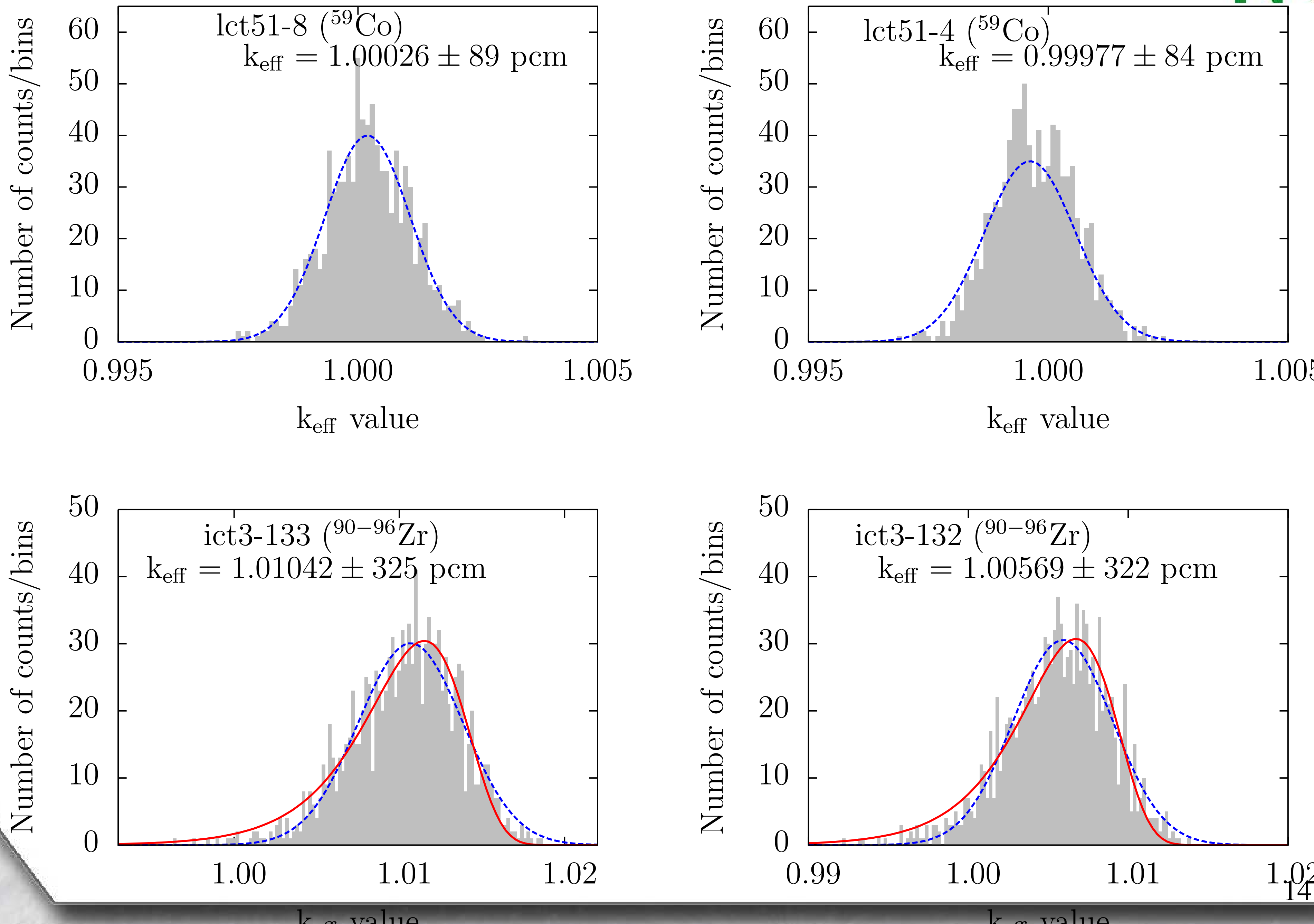




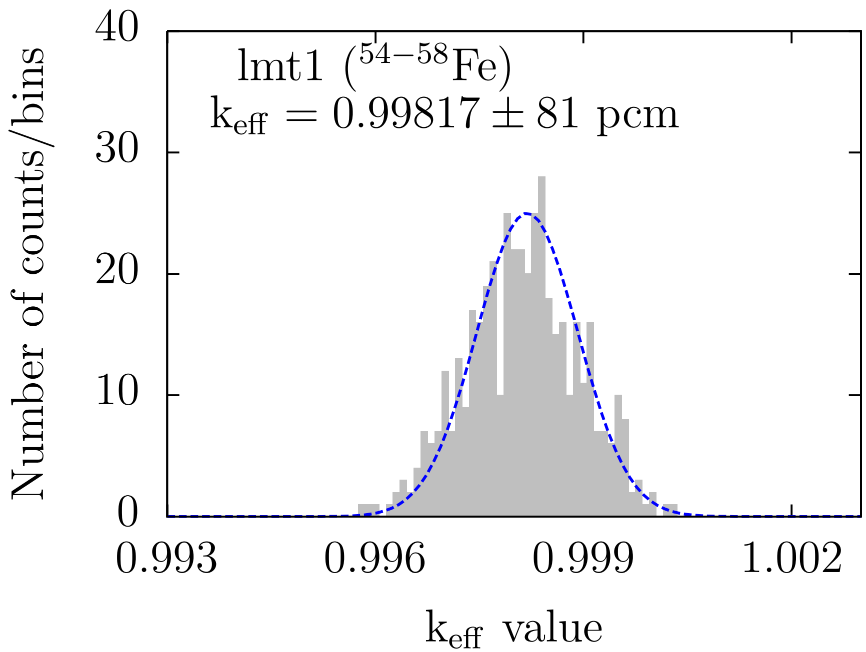
Examples of k_{eff} benchmarks for ^{27}Al and $^{92-100}$Mo

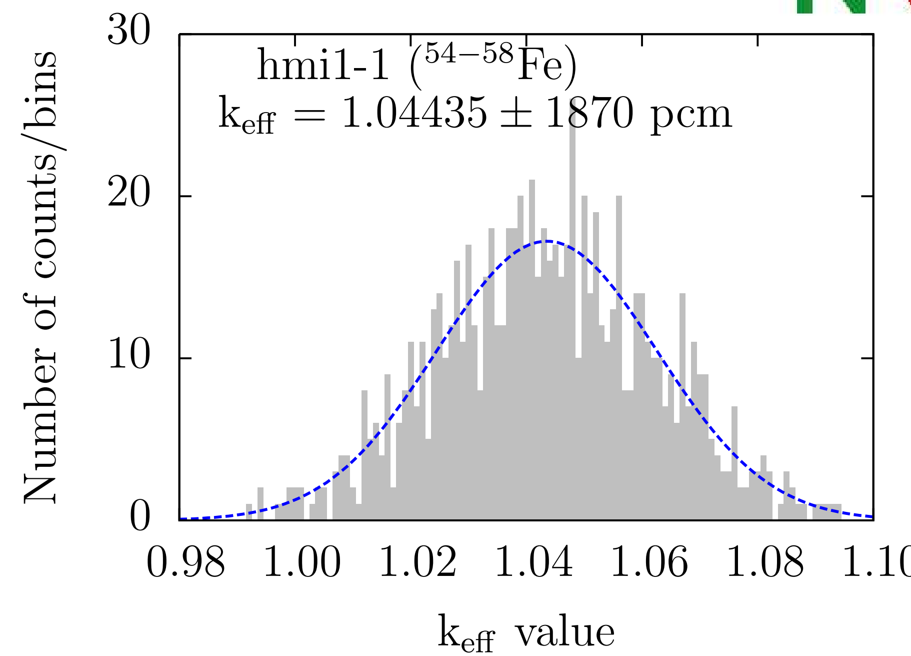


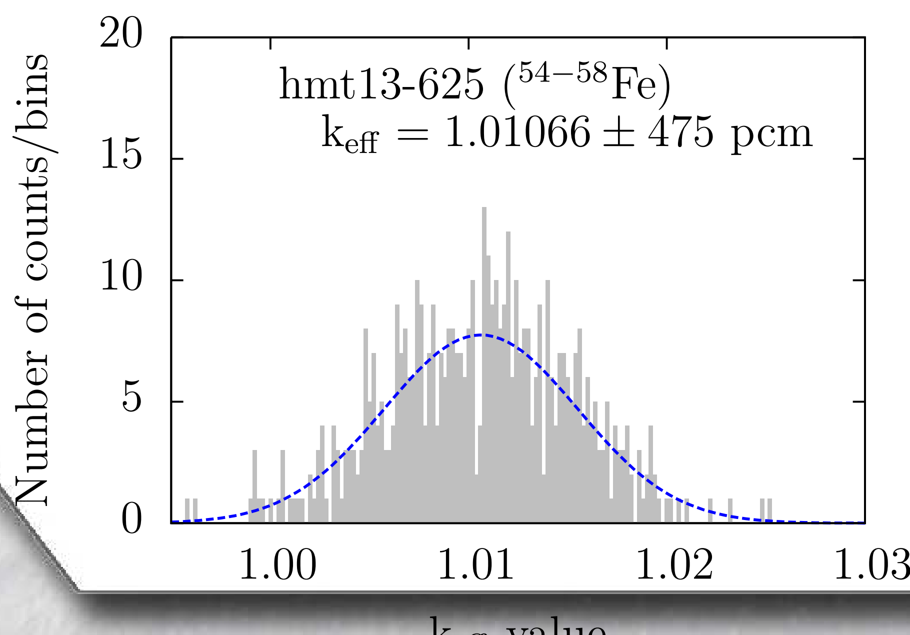
Examples of k_{eff} benchmarks for ^{59}Co and $^{90-96}$Zr

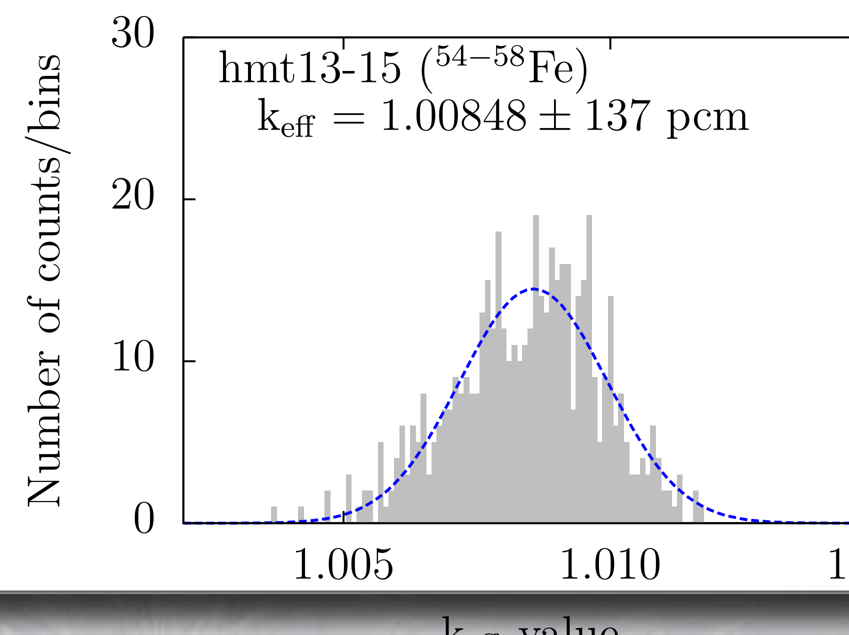


Examples of k_{eff} benchmarks for $^{54-58}$Fe

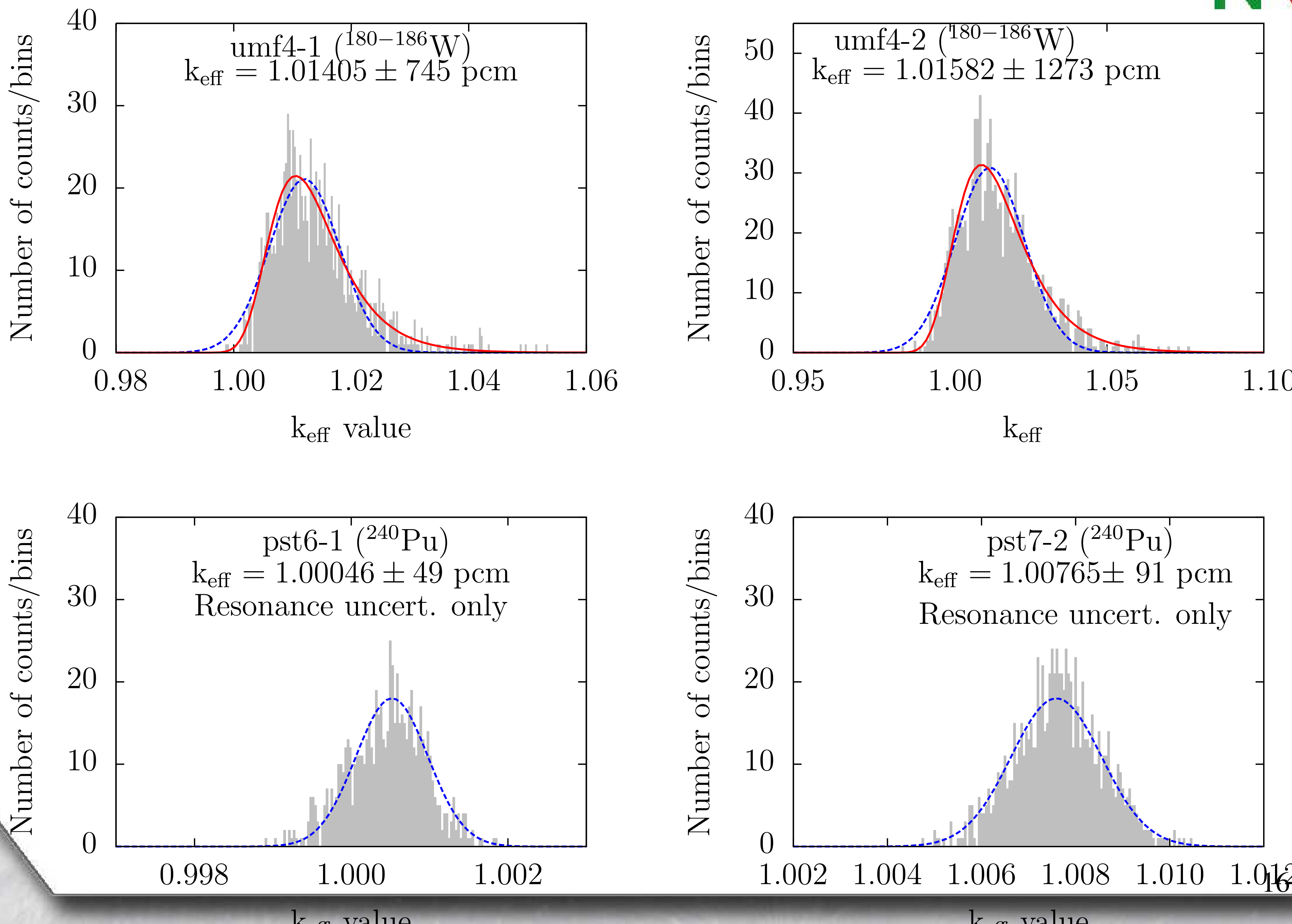




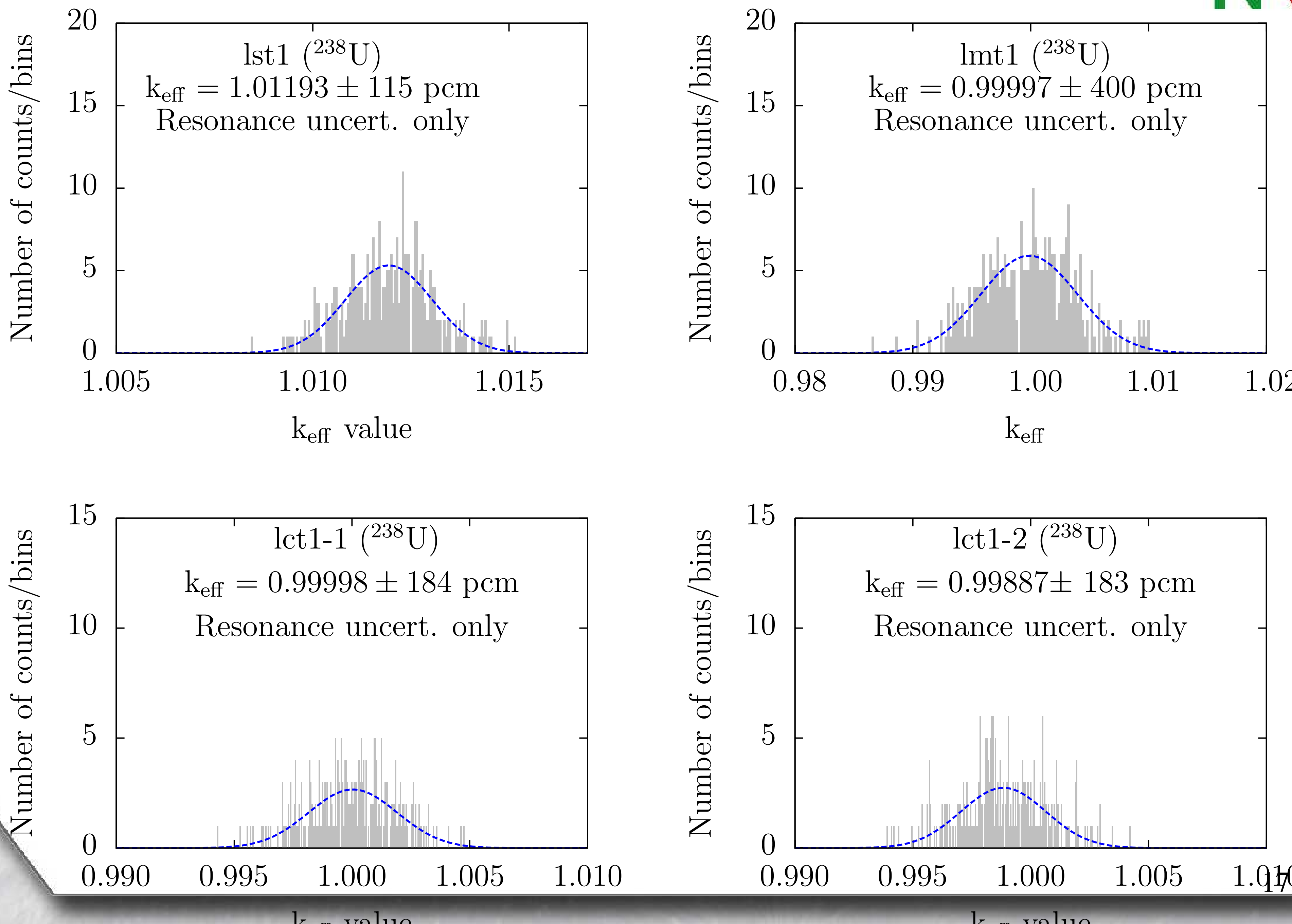




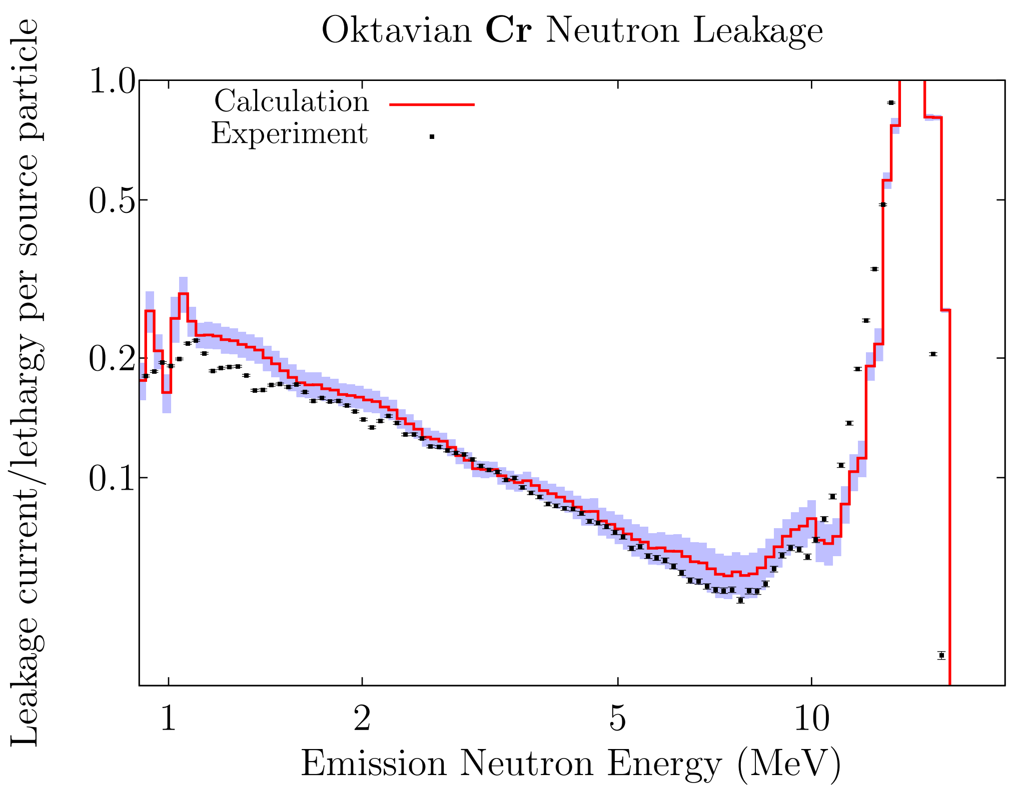
Examples of k_{eff} benchmarks for $^{180-186}$W and ^{240}Pu

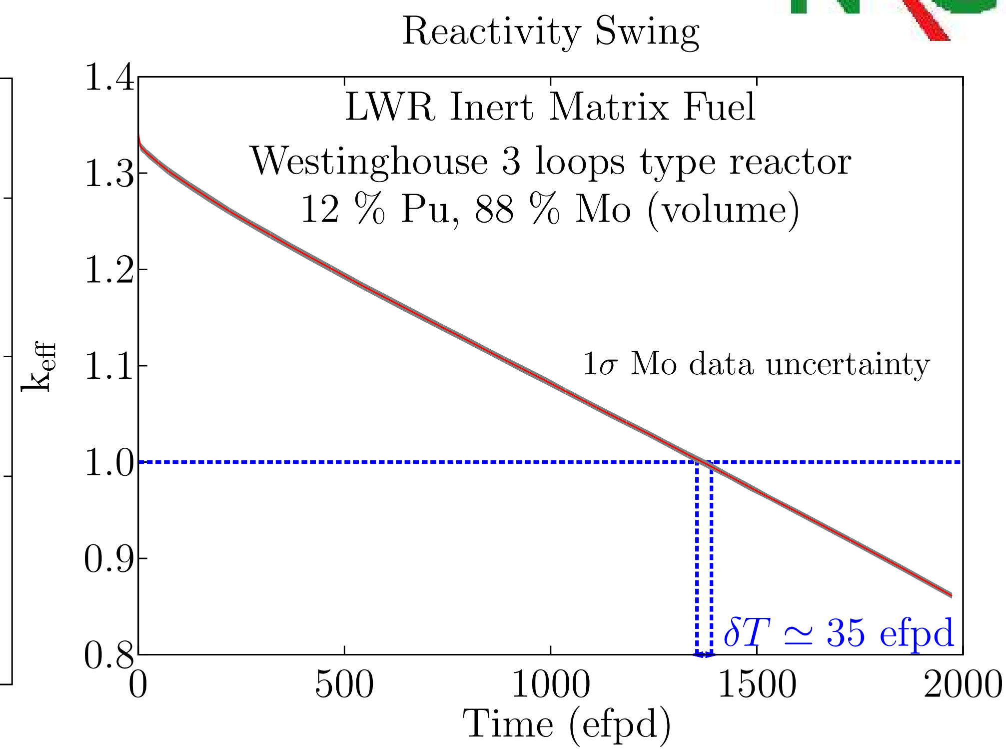


Examples of k_{eff} benchmarks for ^{238}U



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)

Pros and Cons

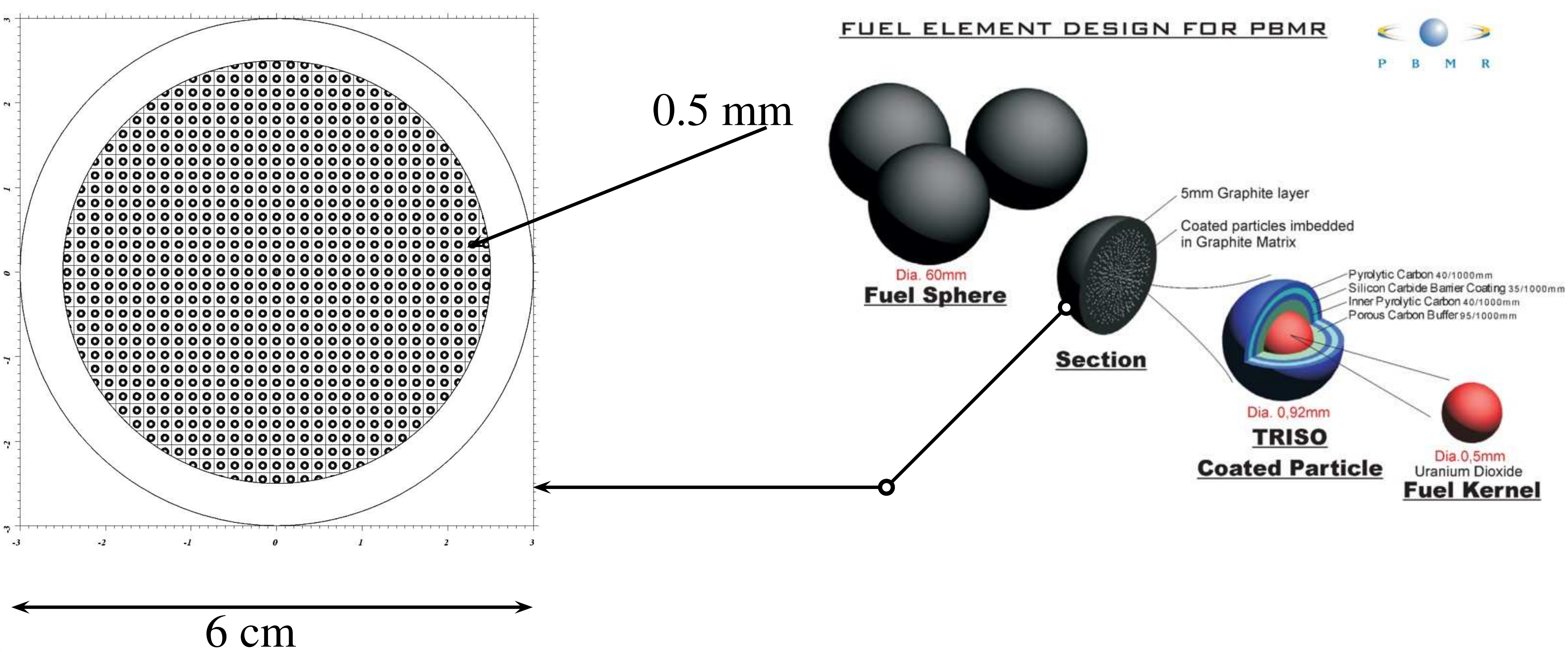
- ☺ + No MF 32-35 (no 2 Gb files) but every possible cross correlation included
- ☺ + No approximation but true probability distribution
- ☺ + Only essential info for an evaluation is stored
- ☺ + No perturbation code necessary, only "essential" codes
- ☺ + Feedback to model parameters
- ☺ + QA
- ☹ - 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) ?

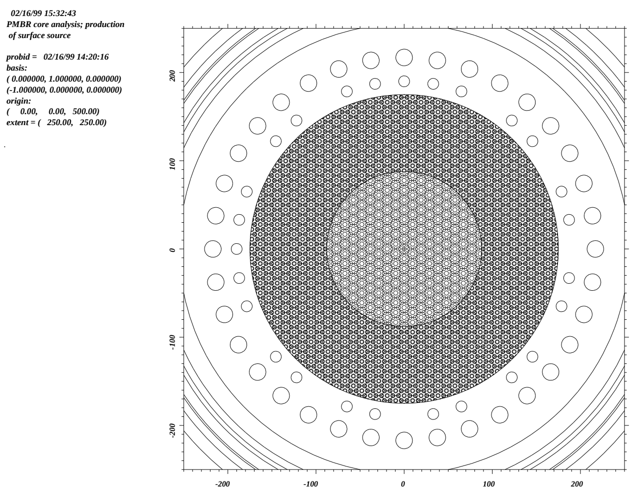
Application to a Pebble Bed Modular Reactor (PBMR)

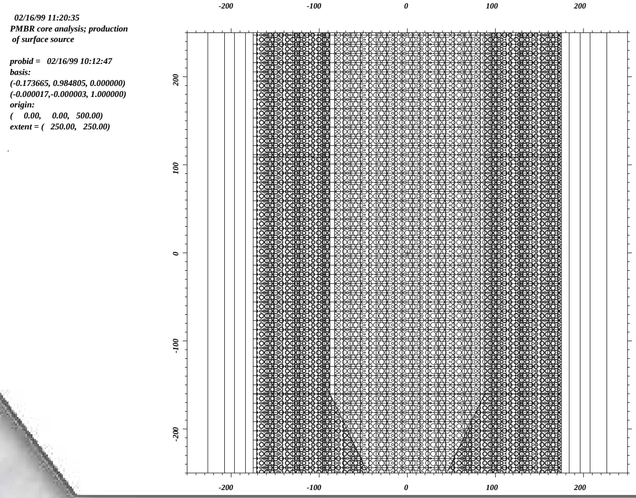
- Model of a fuel pebble
- Fuel particles, surrounded by coating layers, explicitely modelled
- Regular rectangular lattice of fuel particles

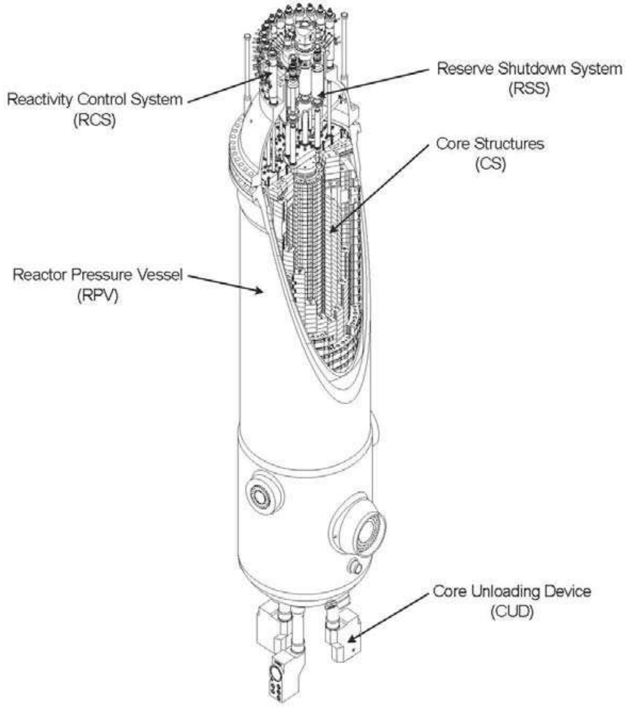


Application to a Pebble Bed Modular Reactor (PBMR)

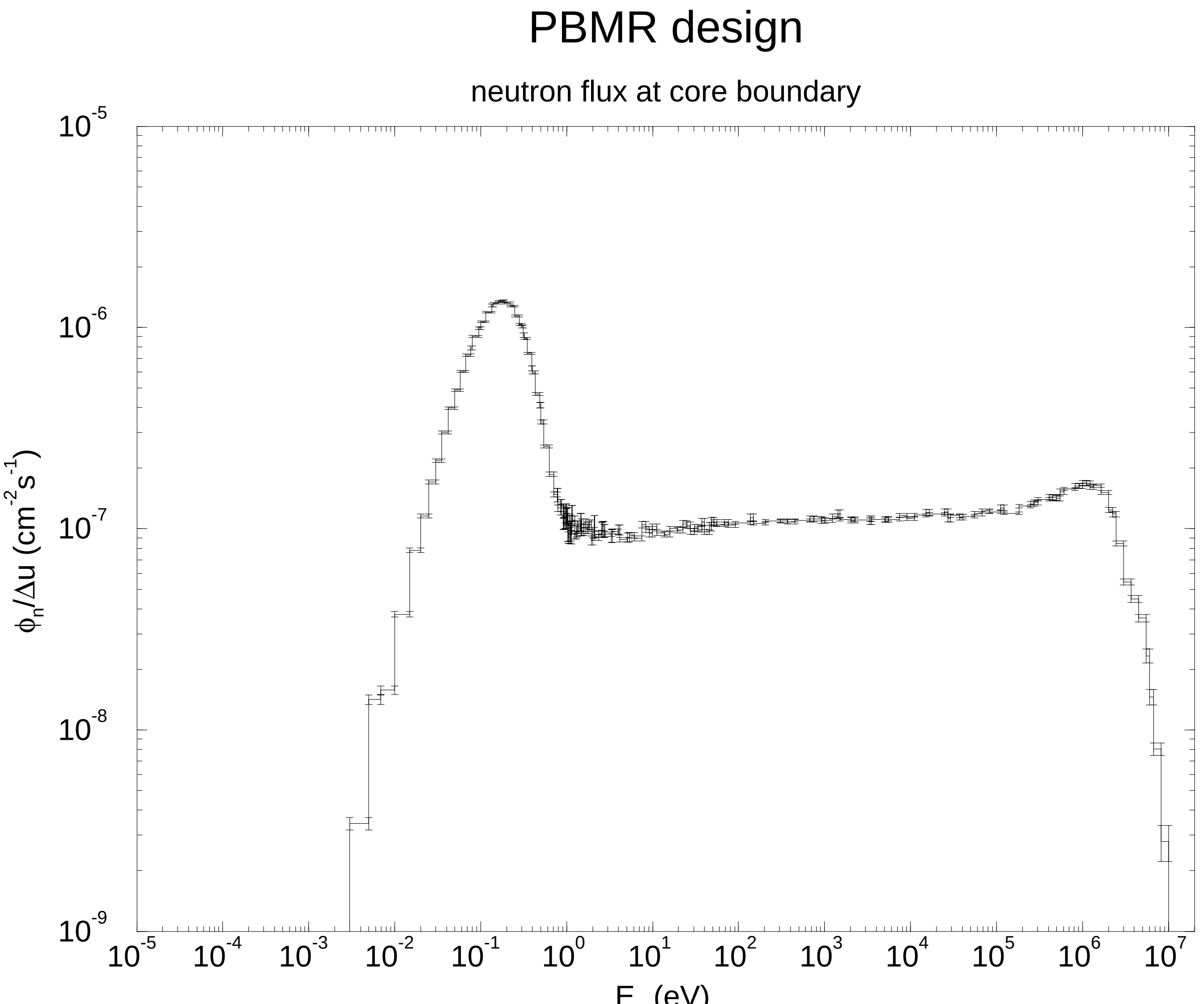
- Hexagonal close packed lattice
- Moderator region consists of homogeneous moderator pebbles as the fuel, reflectors and shields as defined by ESKOM







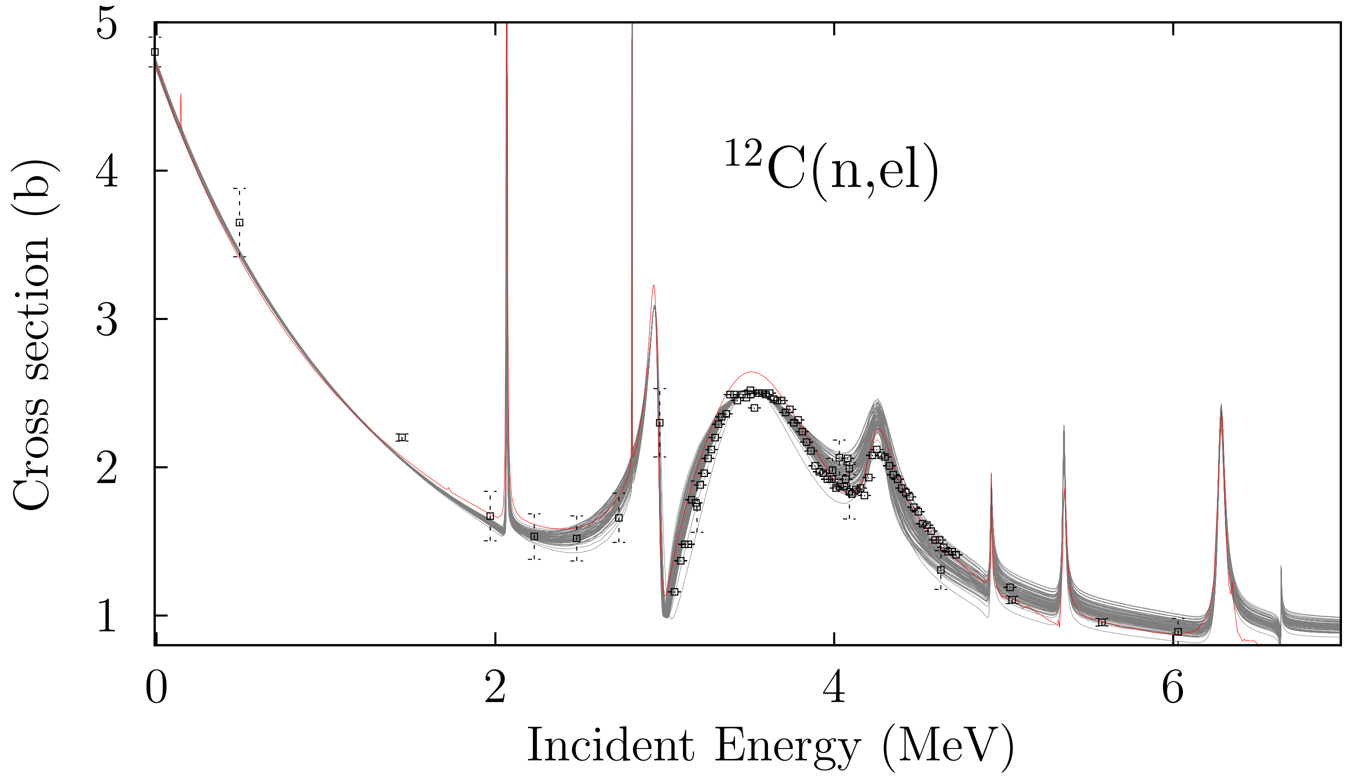
PBMR: Neutron Flux spectrum



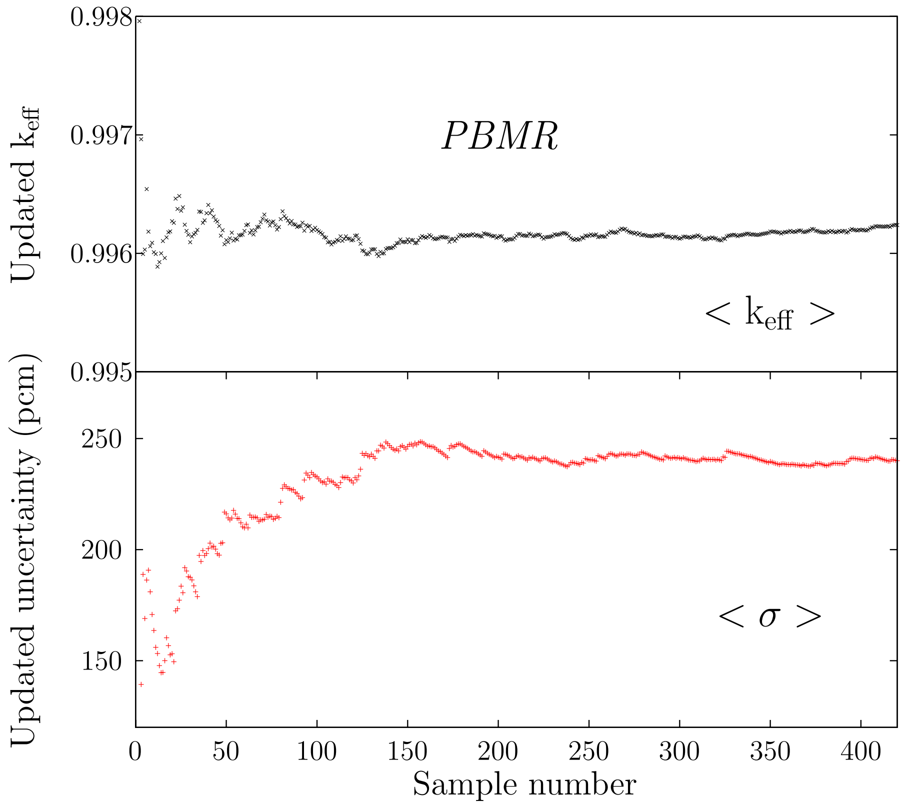
Neutron flux spectrum at the radial core boundary (Almost no neutron above few MeV)

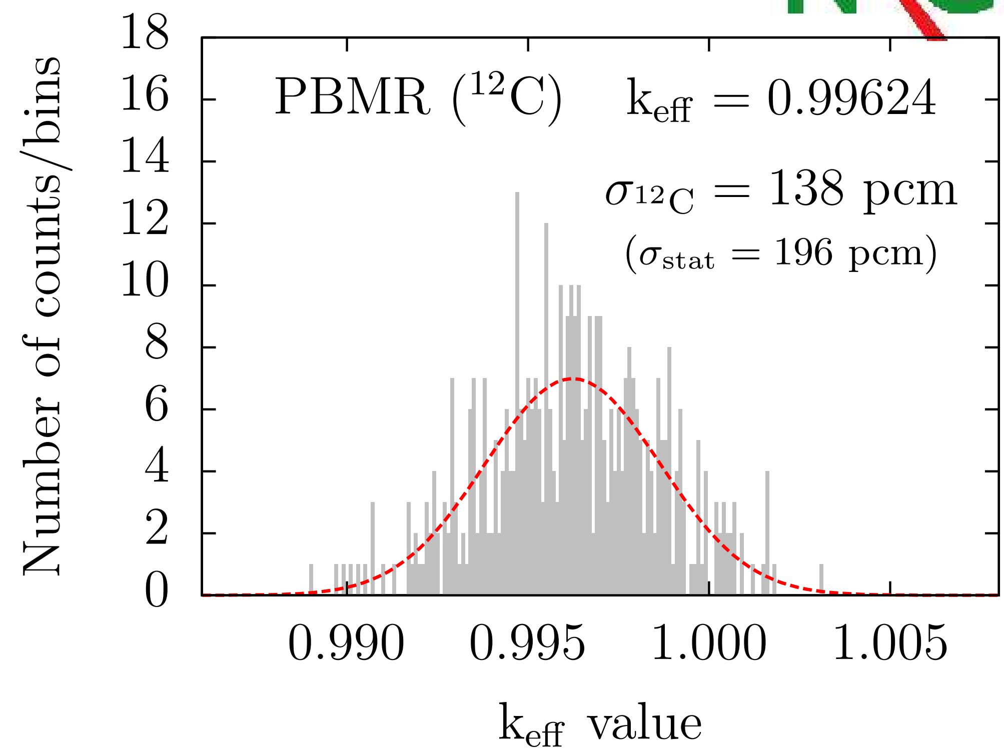
PBMR: ^{12}C nuclear data

- For neutron energy lower than few MeV: only elastic and capture cross sections
- JEFF-3.1: σ_{th} (n,el)= 4.746 ± 0.002b and σ_{th} (n,γ)= 3.53 ± 0.07mb
- 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)

Table 1 (Preliminary)

Benchmark	Isotopes	$k_{eff}/(k_{eff,JEFF-3.1})$ ratio	Statistical uncertainty (pcm)	Uncertainty from nuclear data (pcm)
hmt8d	^{234}U	1.00	46	30
hmt8s	^{234}U	1.00	46	19
hmt9s	^{234}U	1.00	46	22
hmt10-15	^{234}U	1.00	45	12
hmt10-7	^{234}U	1.00	45	32
hmt18d	^{234}U	0.99	46	48
hmt18s	^{234}U	1.00	46	52
hmt14s	^{234}U	1.00	48	35
pst6-1	^{240}Pu	1.00	40	27
pst6-2	^{240}Pu	1.00	39	31
pst6-3	^{240}Pu	1.00	40	23
pst7-2	^{240}Pu	1.00	49	76
pst7-3	^{240}Pu	1.00	49	71
mmf11-1	^{241}Am	1.00	37	< 37

Table 2 (Preliminary)

Benchmark	Isotopes	$k_{eff}/(k_{eff,JEFF-3.1})$ ratio	Statistical uncertainty (pcm)	Uncertainty from nuclear data (pcm)
lst-1	^{238}U	1.00	26	108
lmt-1	^{238}U	1.00	61	405
lct1-1	^{238}U	1.00	69	176
lct1-2	^{238}U	1.00	69	165
lct2-1	^{238}U	1.00	79	110
lct2-2	^{238}U	1.00	80	117
lct2-3	^{238}U	1.00	79	130
lct2-4	^{238}U	1.00	78	100
lct2-5	^{238}U	1.00	77	105
lct3-1	^{238}U	1.00	34	132
lct3-2	^{238}U	1.00	39	134
lct3-3	^{238}U	1.00	39	125
lct3-4	^{238}U	1.00	38	137
lct3-5	^{238}U	1.00	38	141
lct3-6	^{238}U	1.00	36	153

Table 3 (Preliminary)

Benchmark	Isotopes	$k_{eff}/(k_{eff,JEFF-3.1})$ ratio	Statistical uncertainty (pcm)	Uncertainty from nuclear data (pcm)
hmf7-32	^{19}F	1.00	67	465
hmf7-33	^{19}F	1.00	68	734
hmf7-34	^{19}F	1.00	70	943
hst39-1	^{19}F	1.00	95	1058
hst39-2	^{19}F	1.01	97	1003
hst39-3	^{19}F	1.01	96	961
hst9-2	^{19}F	1.00	24	59
hst9-3	^{19}F	1.00	24	39
lst1	^{19}F	1.00	85	116
imf10-1	$^{28-30}Si$	0.99	32	25
lct1-1	$^{28-30}Si$	1.00	69	49
hmf5-2	$^{28-30}Si$	1.00	72	20
hmf5-3	$^{28-30}Si$	1.00	76	< 76
hmf5-4	$^{28-30}Si$	1.00	78	< 78
hmf5-5	$^{28-30}Si$	1.00	71	18