Nuclear data uncertainty propagation with Monte Carlo methods

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Nuclear Research and Consultancy Group,

NRG, Petten, The Netherlands

GRS Garching, July 2013

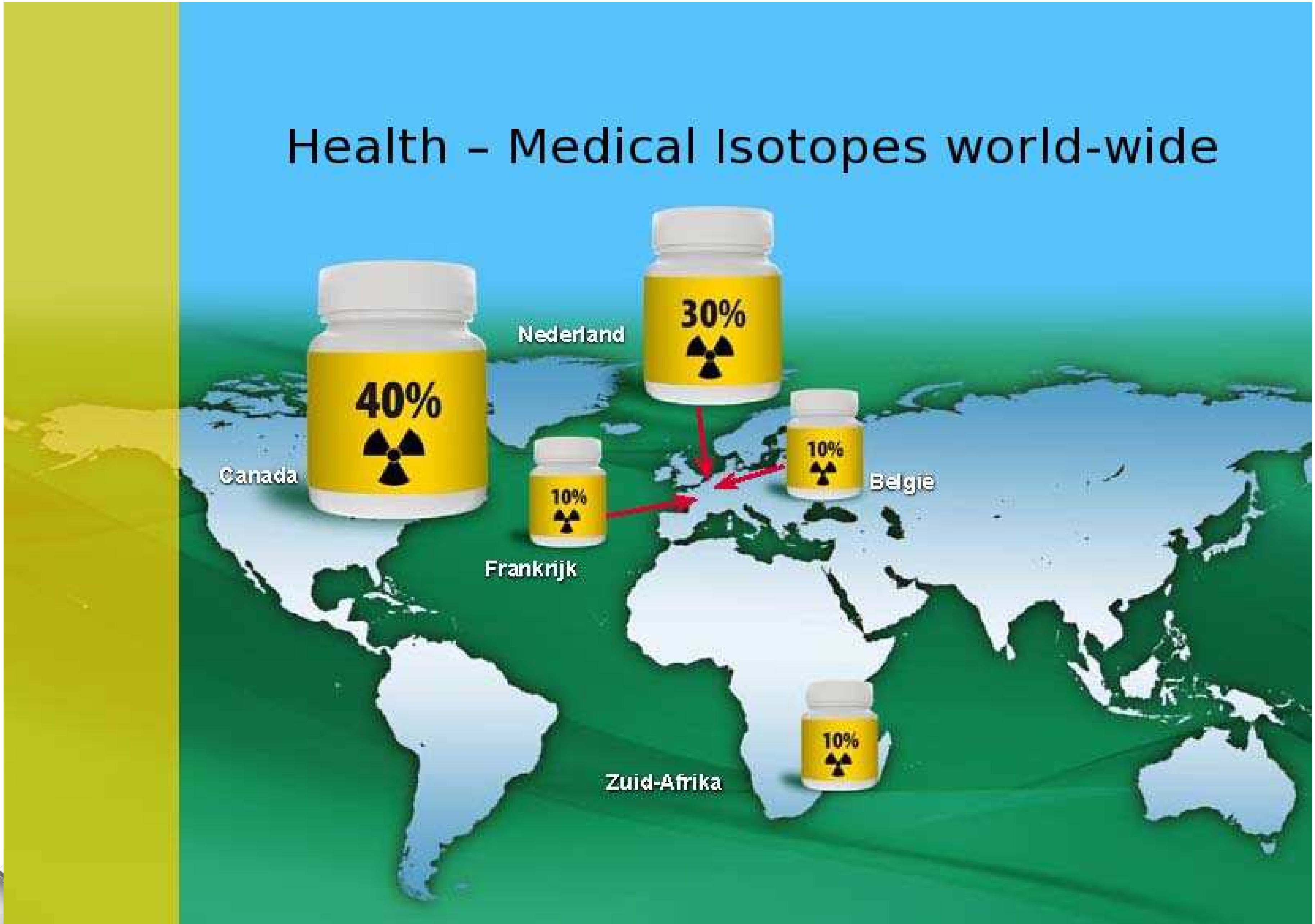
Contents

All slides can be found at:
ftp://ftp.nrg.eu/pub/www/talys/bib_rochman/presentation.html.

Who are we ?

- NRG: a leading nuclear sector service provider
- Over 50 years experience in nuclear technology
- Over 400 employees (10 in R&D reactor physics and simulations)
- Turnover approximately Meuros 60 / per year
- High Flux Reactor, Hot Cell Laboratories and Radiological labs

Who are we ?



Health – Medical Isotopes world-wide
Nederland
30%
40%
Canada
10%
Belgie
10%
Frankrijk
Zuid-Afrika
10%

What are nuclear data ?

The term ”nuclear data” can have different meaning,

- dusty books, constants, mature field, code inputs,
- list, Schrodinger equation, unexciting...
- but this is not ! (I’m going to prove that)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U.S. News

U.S., Russia exchange nuclear data

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President Dimitri Medvedev (L) of Russia and U.S. President Barack Obama hold a bilateral meeting at the United Nations in New York on September 23, 2009. UPI/Olivier Douliery/Pool

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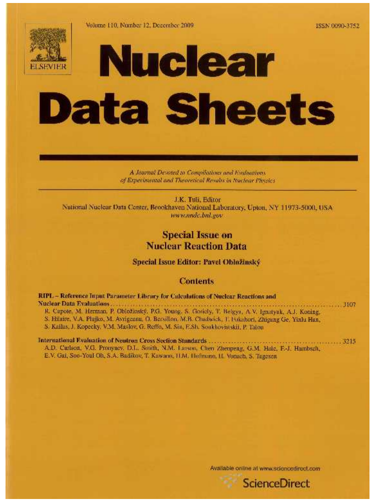


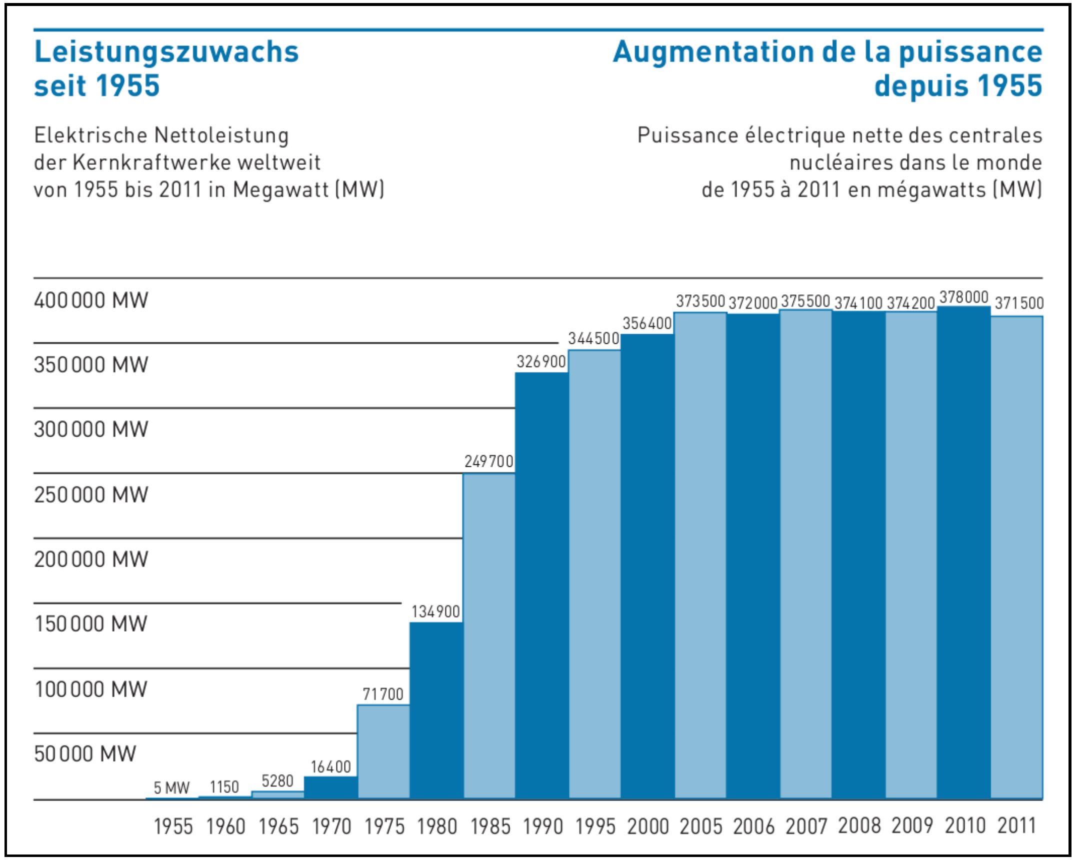
Why are nuclear data important ? (Part 1)

Better nuclear data can help for:

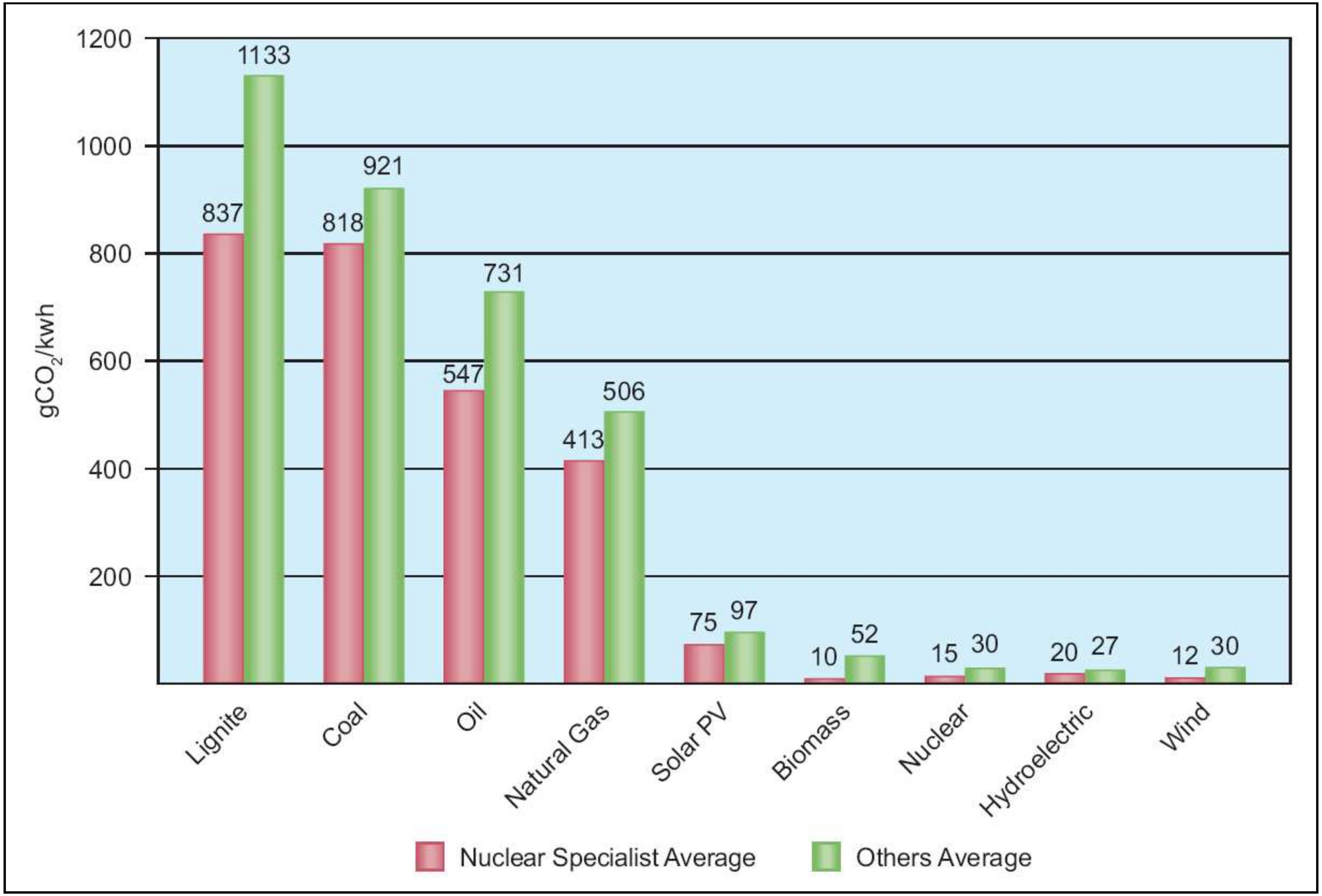
- ▶ safety margins, fuel storage,
- ▶ life-time extension,
- ▶ cost reduction in design of new systems,
- ▶ isotope production,
- ▶ safety of people (shielding),
- ▶ waste transmutation,
- ▶ development of future systems.

Better nuclear data have a limited effect on:

- ◀ current reactor operation,
- ◀ current reactor safety,...
- ◀ accident simulation,
- ◀ proliferation,
- ◀ Chernobyl, TMI, Fukushima.



Why are nuclear data important ? (Part 2)



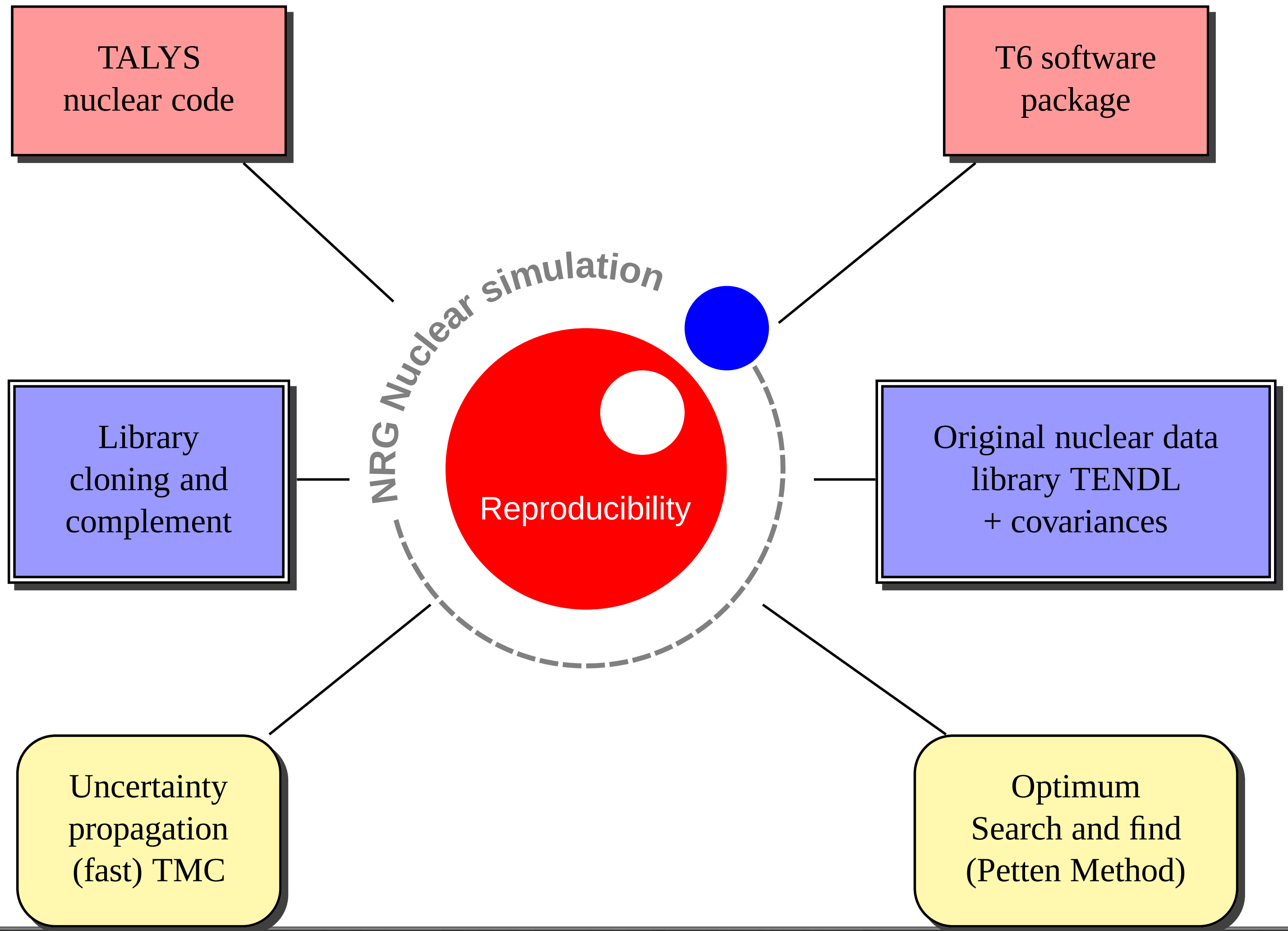
Source: World Nuclear Association Report

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

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

Our mission: improve nuclear simulations



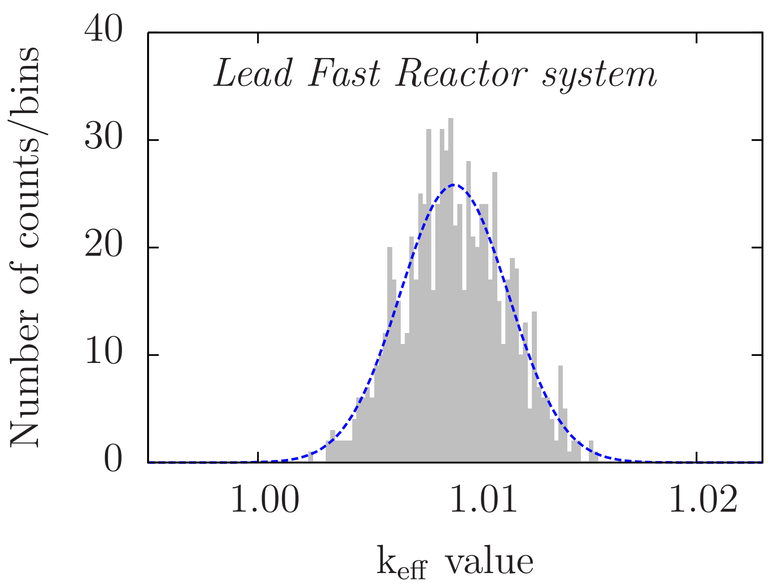
2008: Total Monte Carlo (TMC)

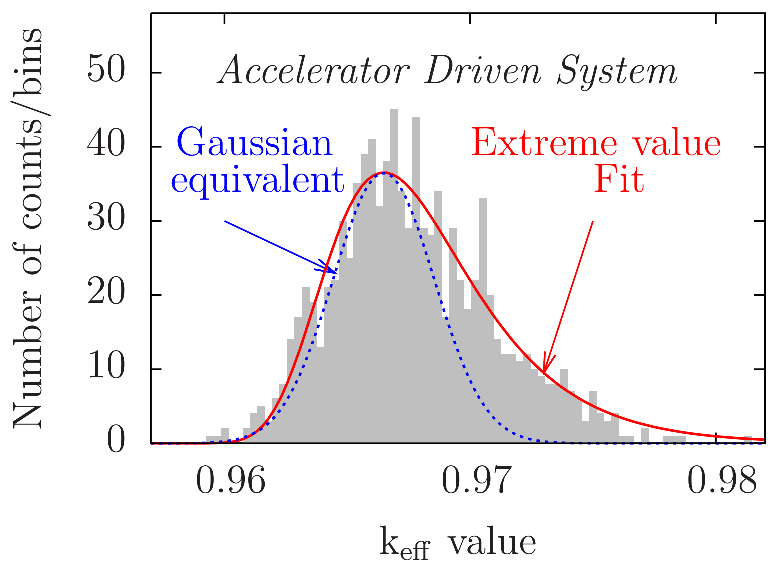
Control of nuclear data (TALYS system)
+ processing (NJOY)
+ system simulation (MCNP/ERANOS/CASMO...)

1000 times

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.

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



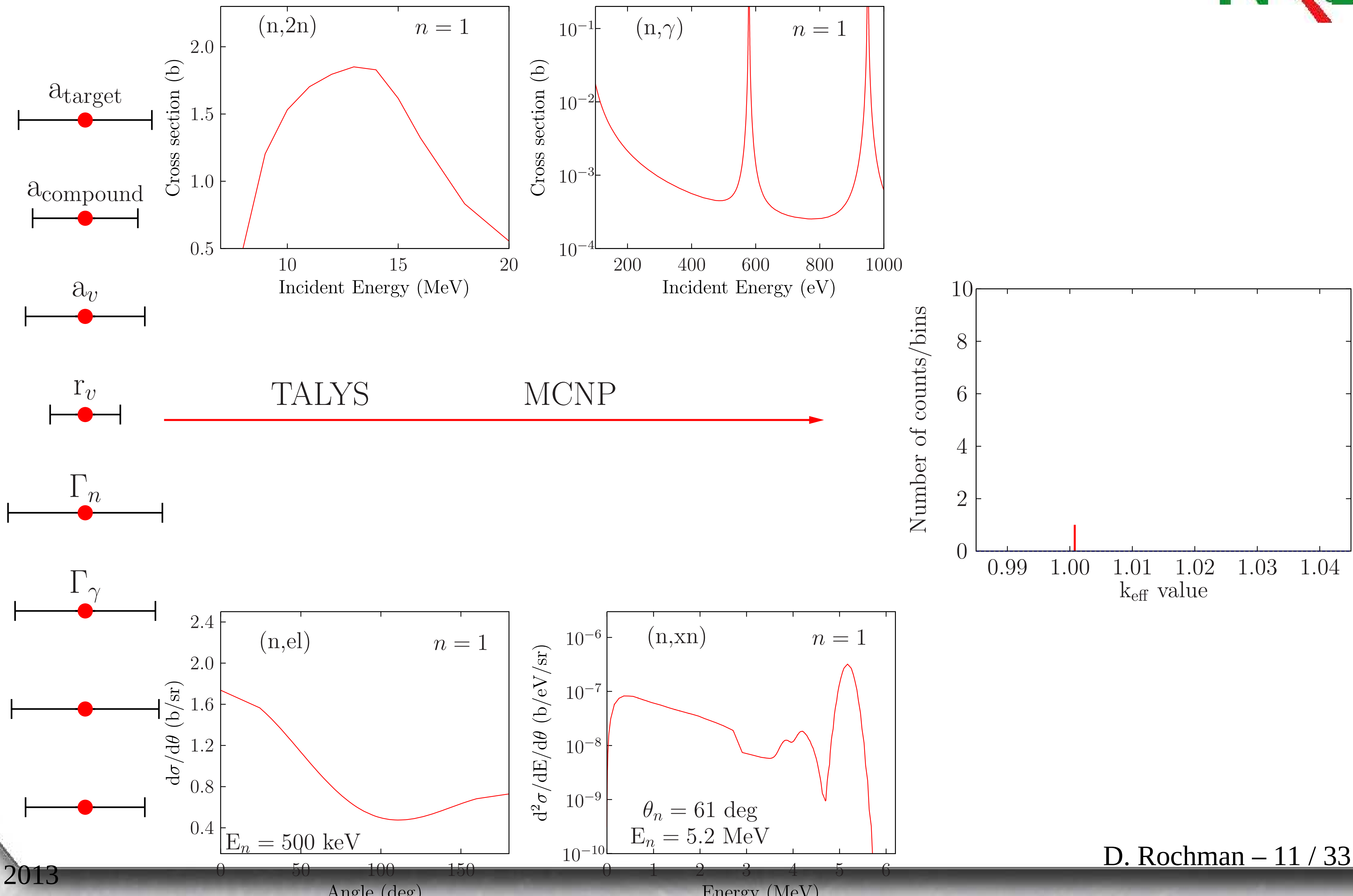


"Towards sustainable nuclear energy: Putting nuclear physics to work",
A.J. Koning and D. Rochman, ANE 35 (2008) 2024.

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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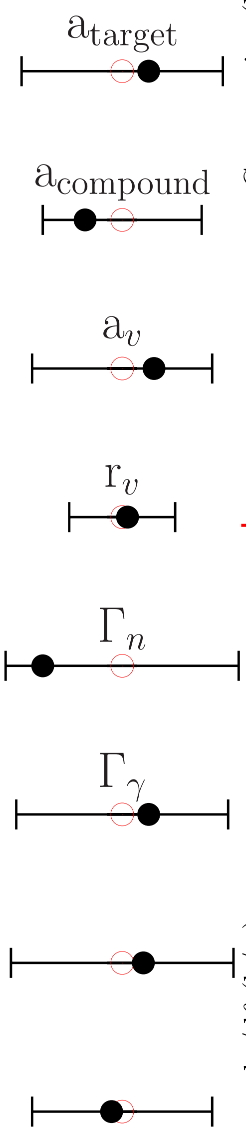

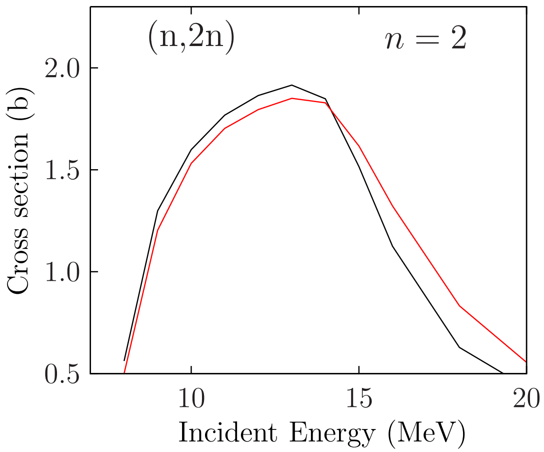

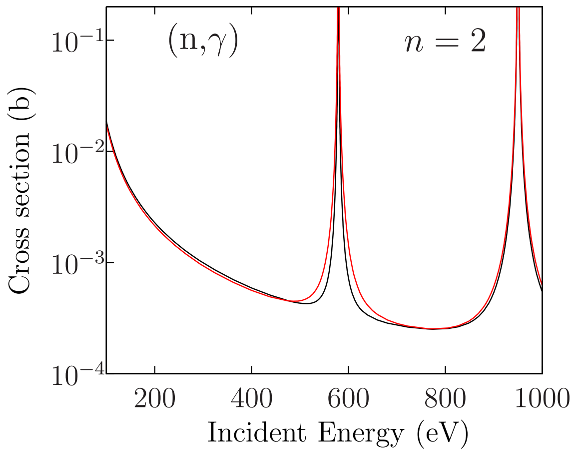

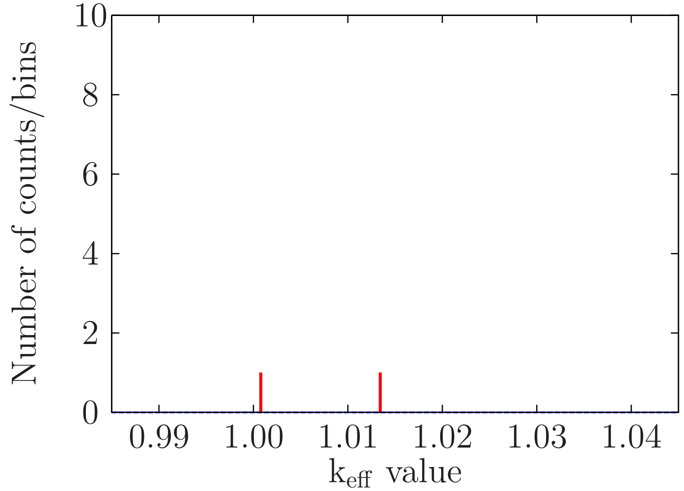

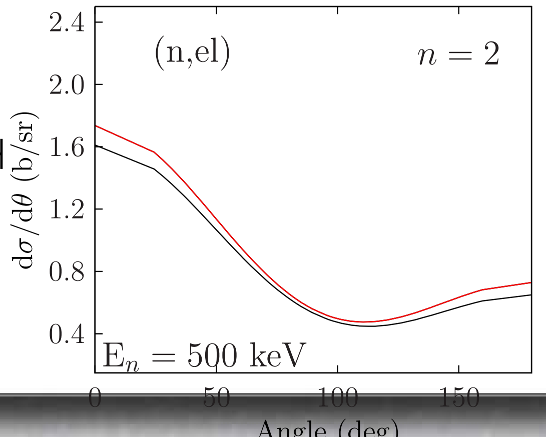

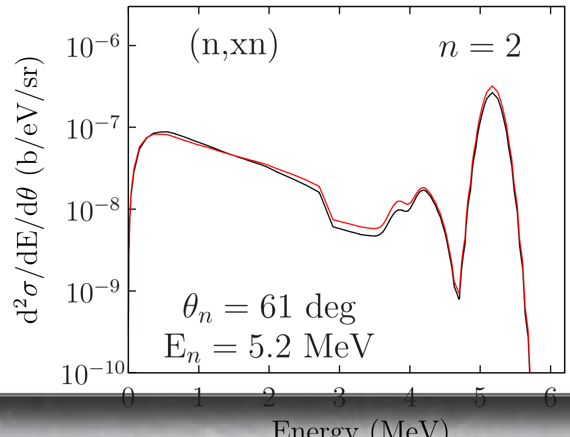

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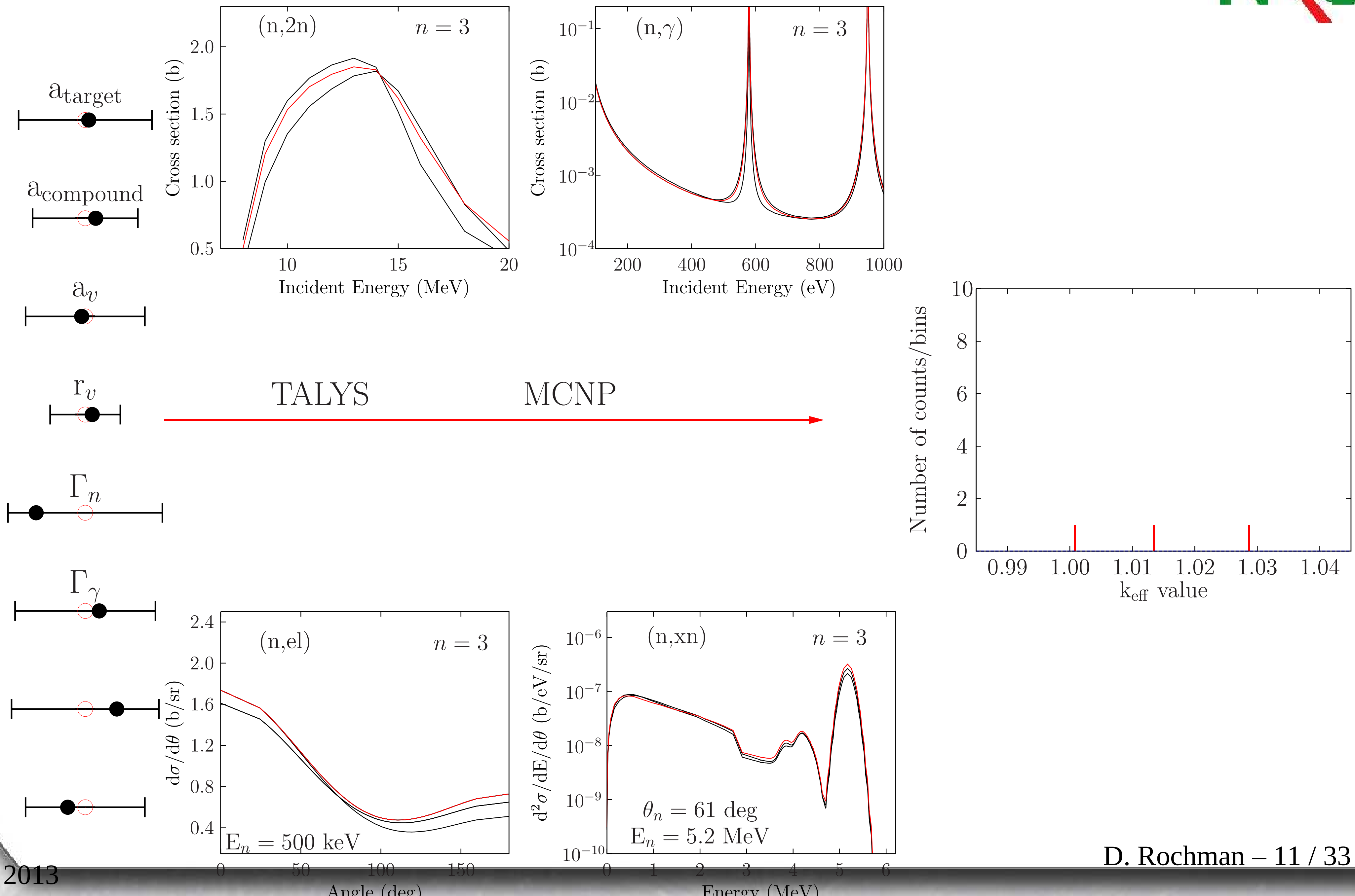

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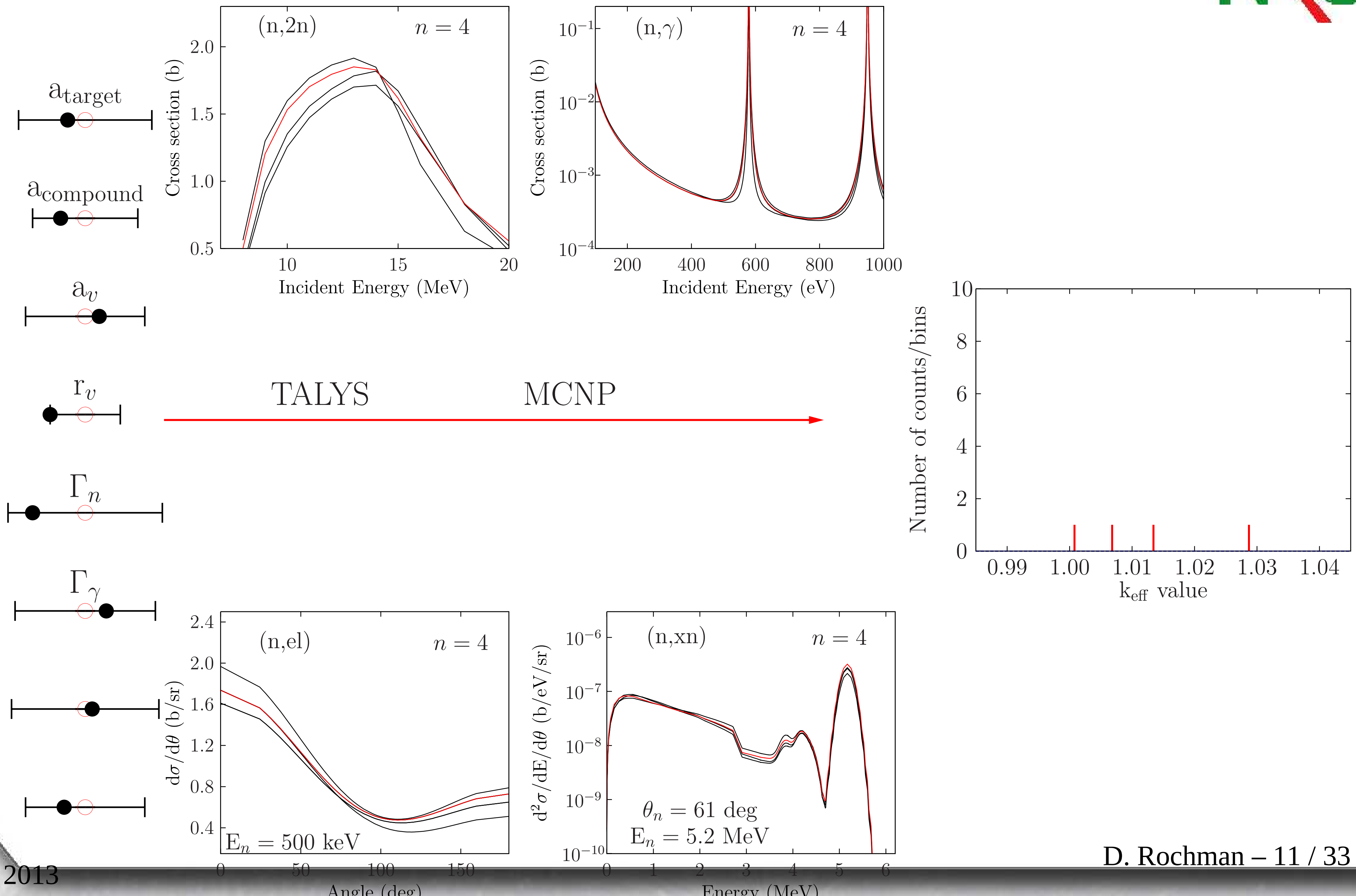

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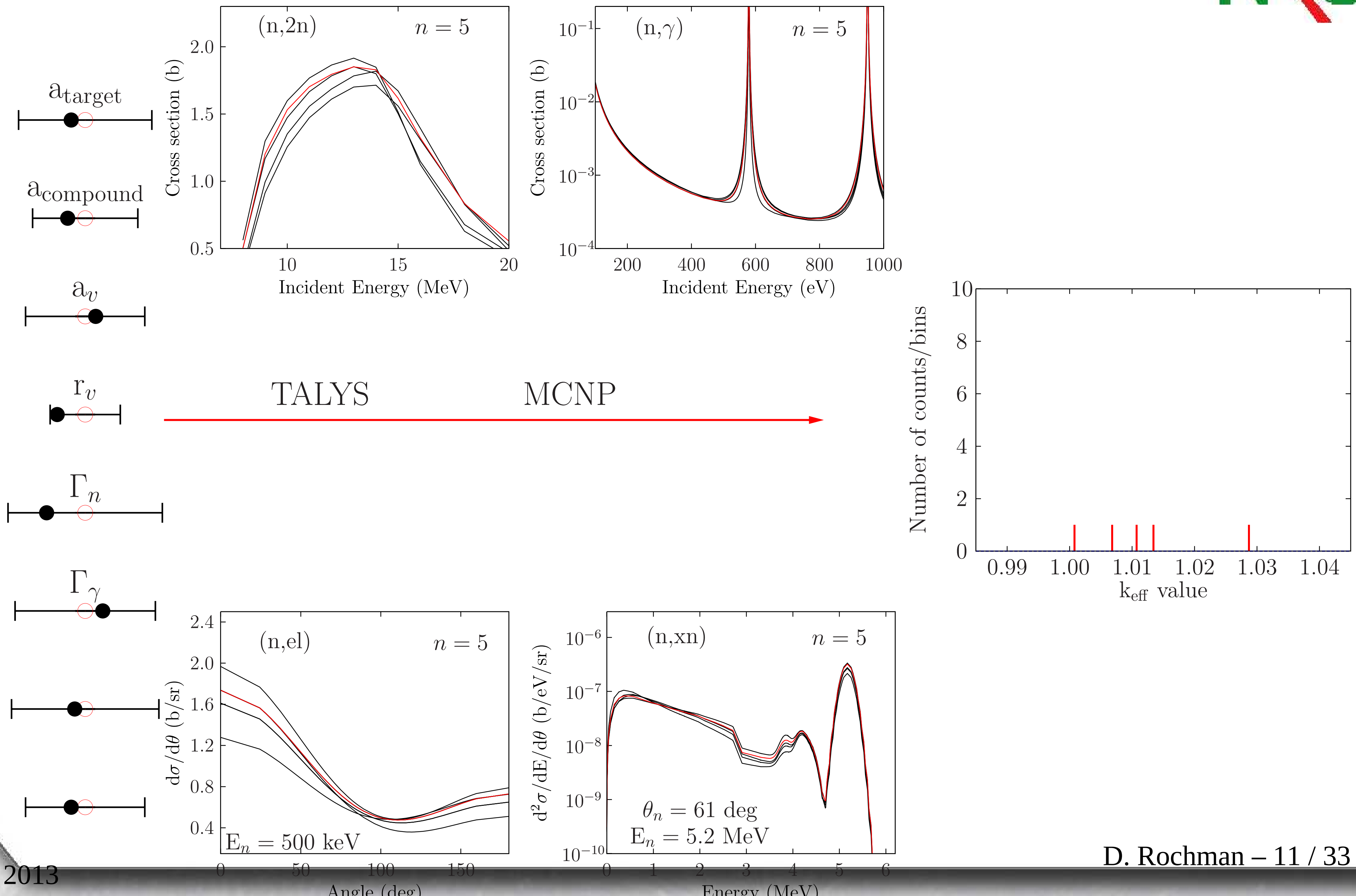

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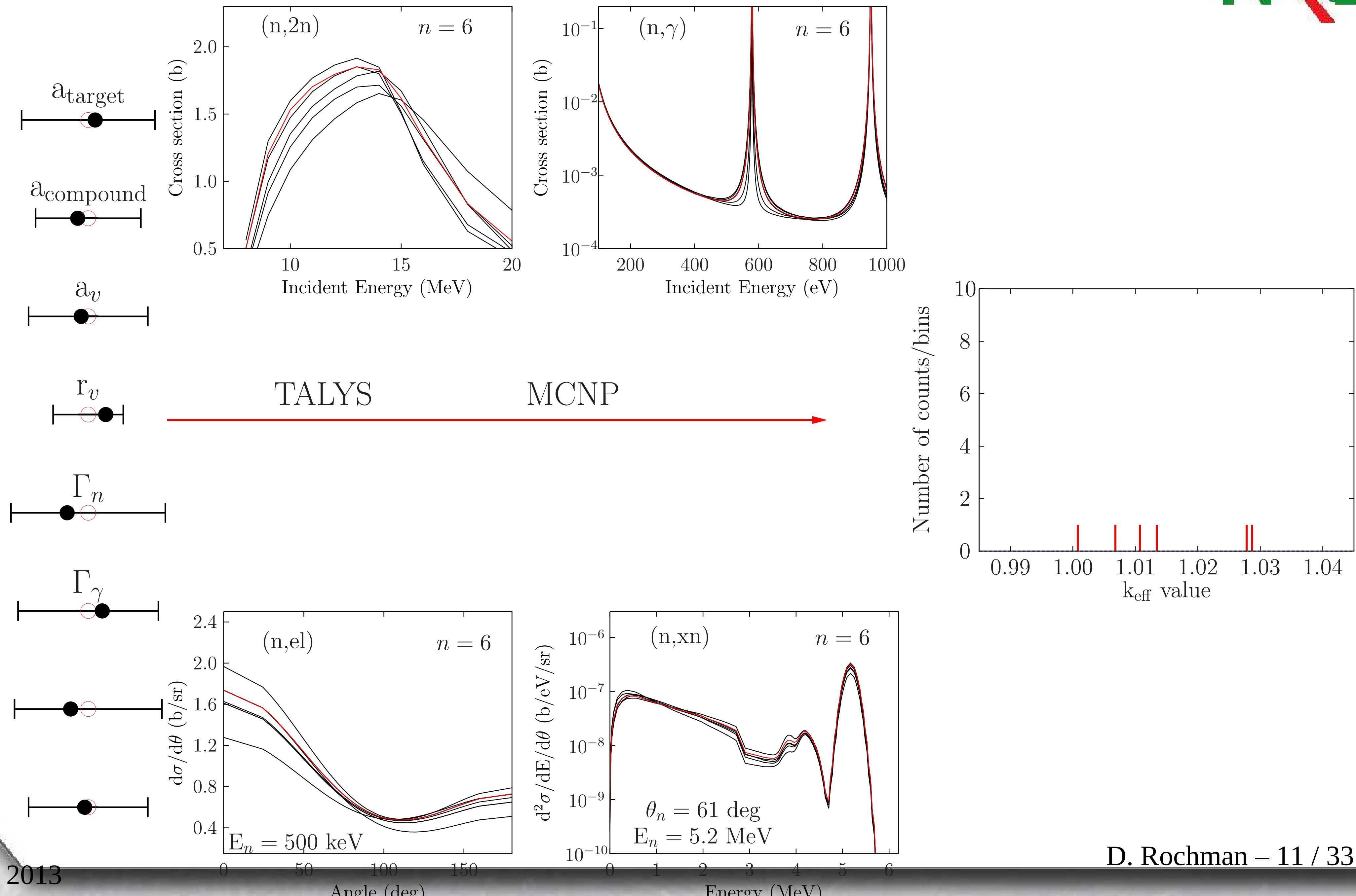

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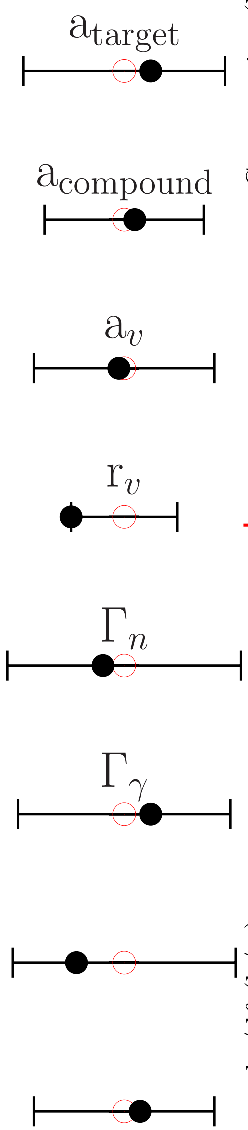

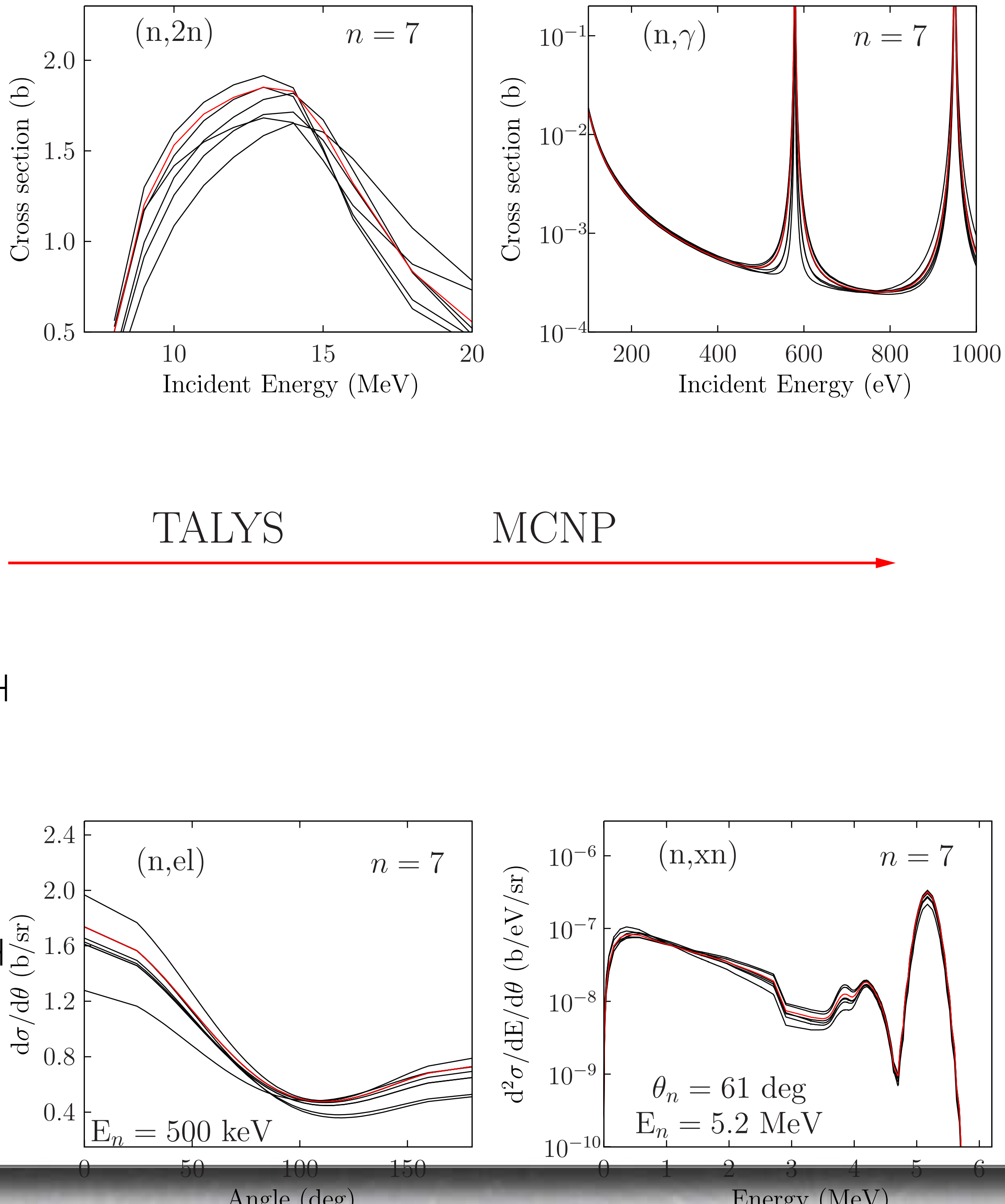

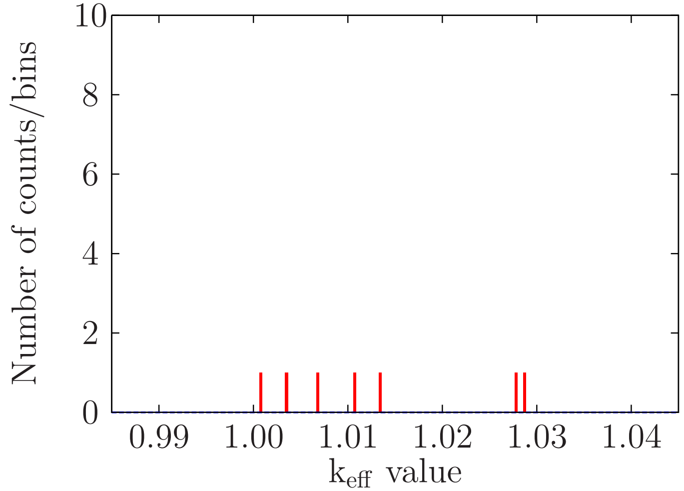

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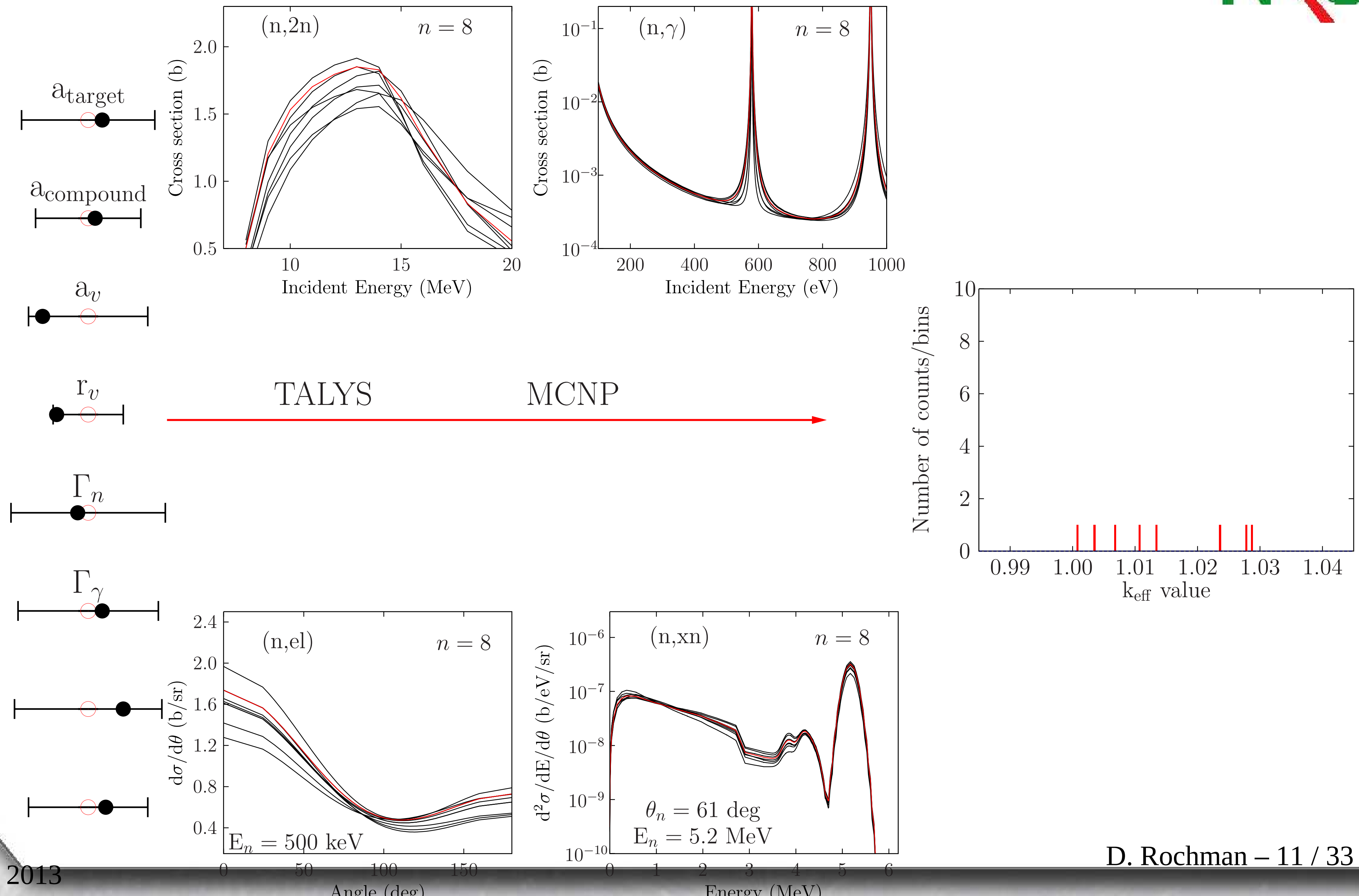

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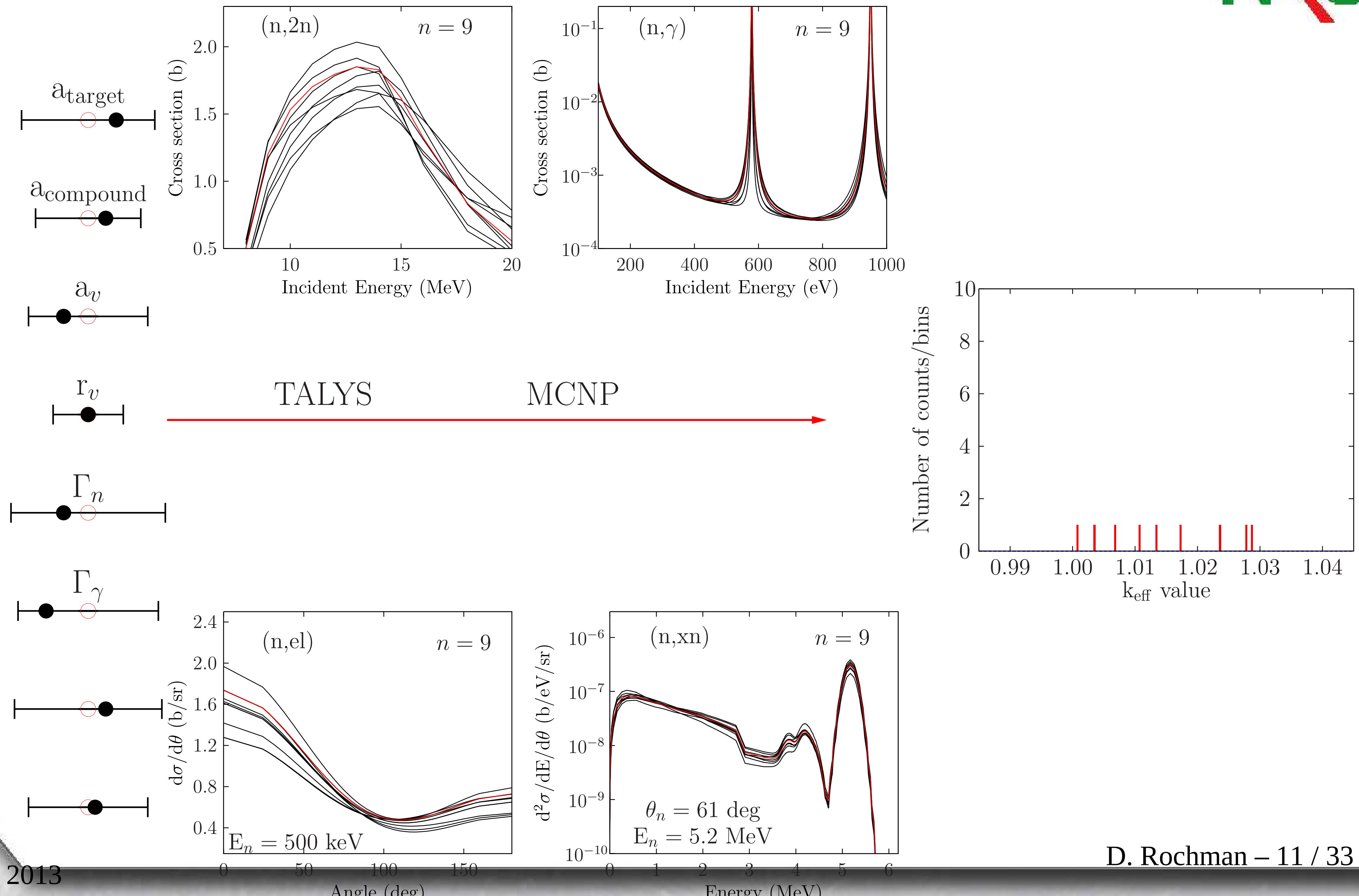

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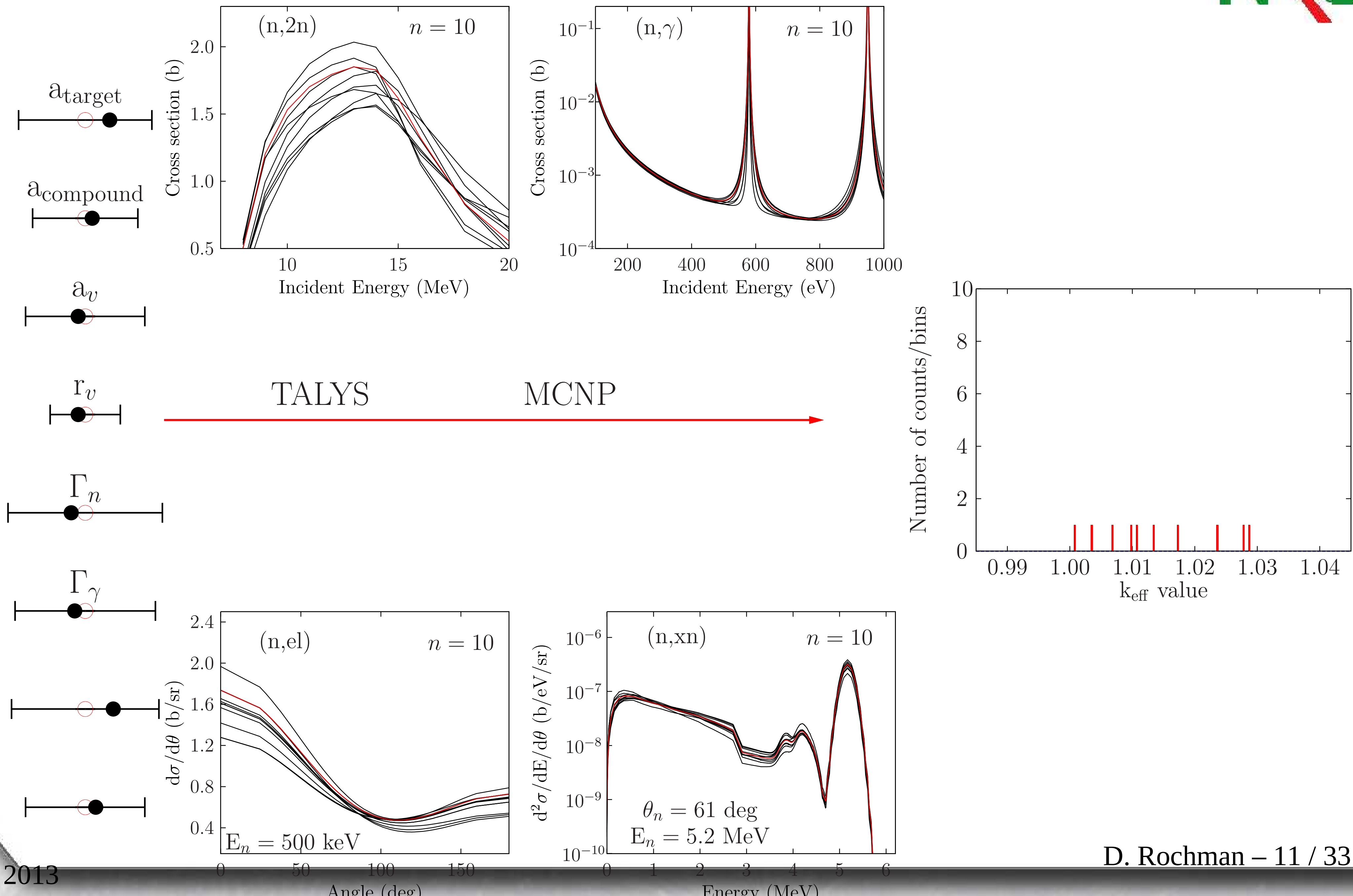

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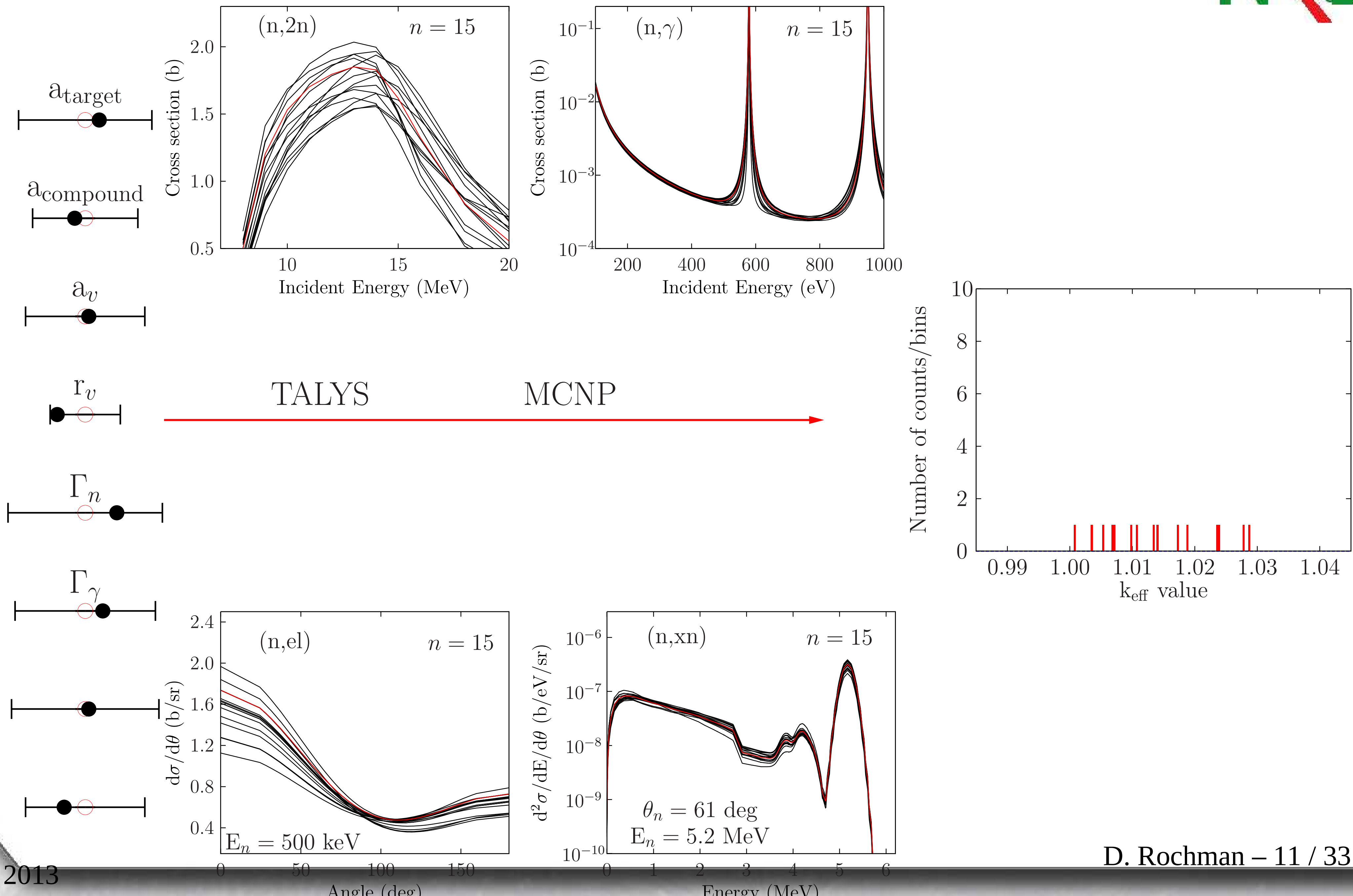

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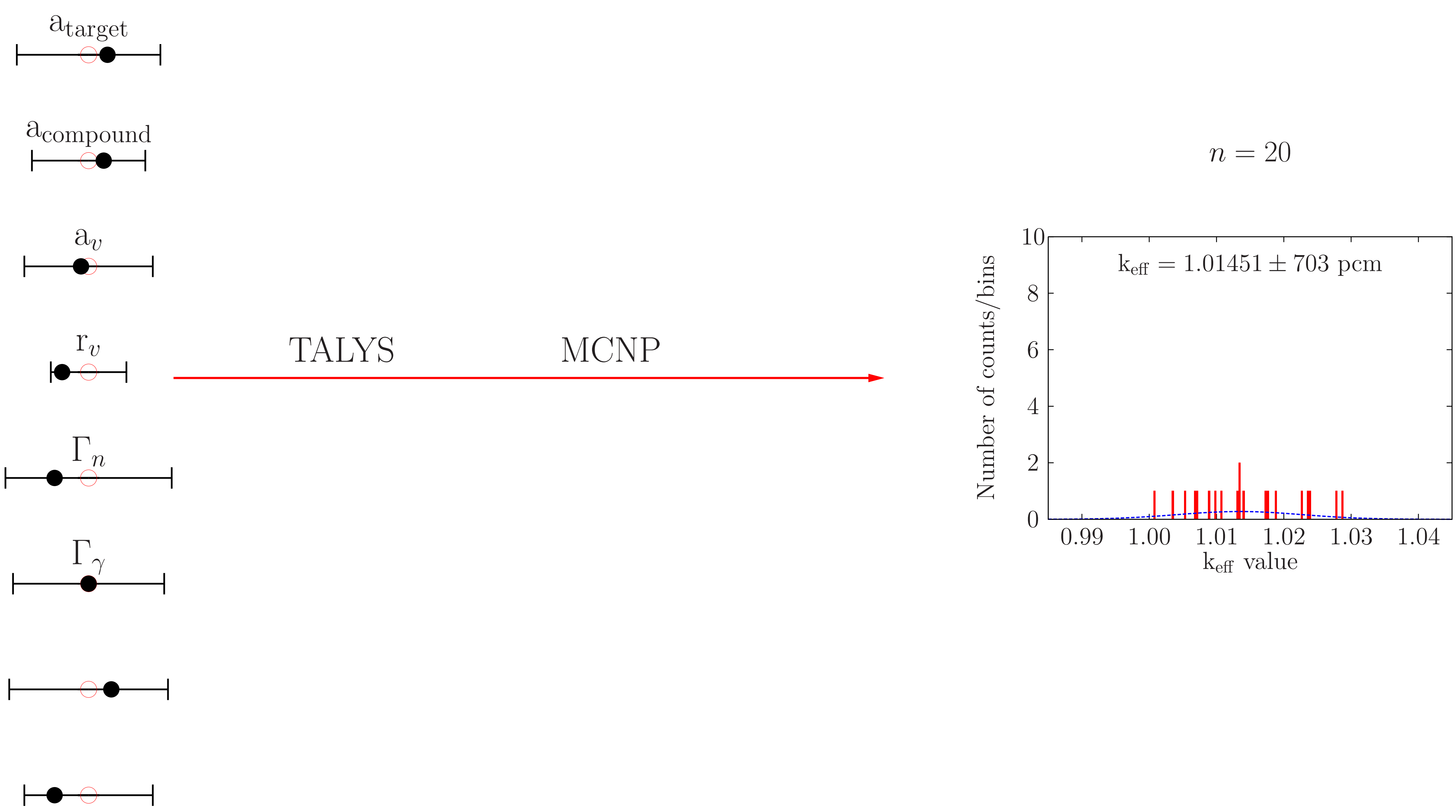

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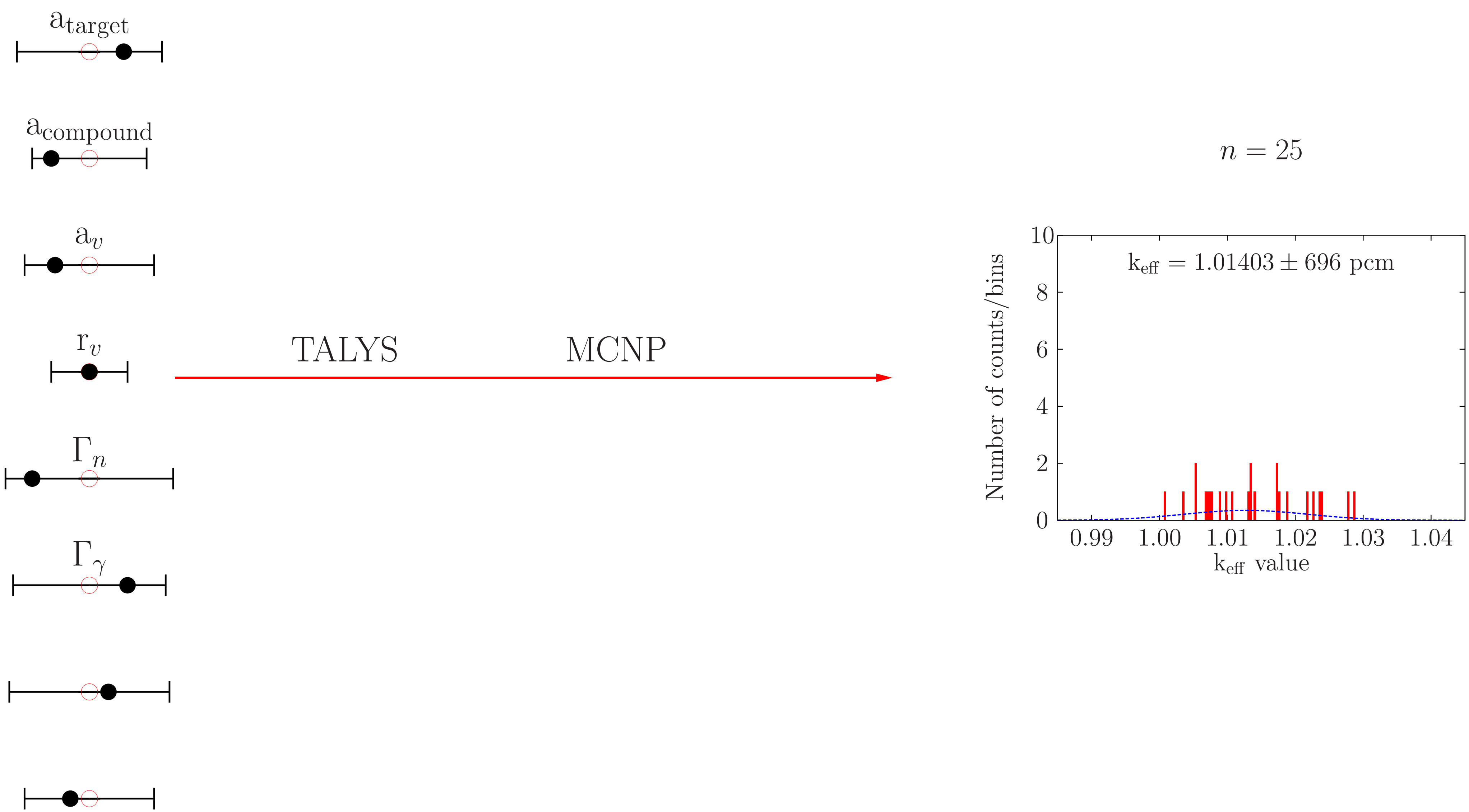

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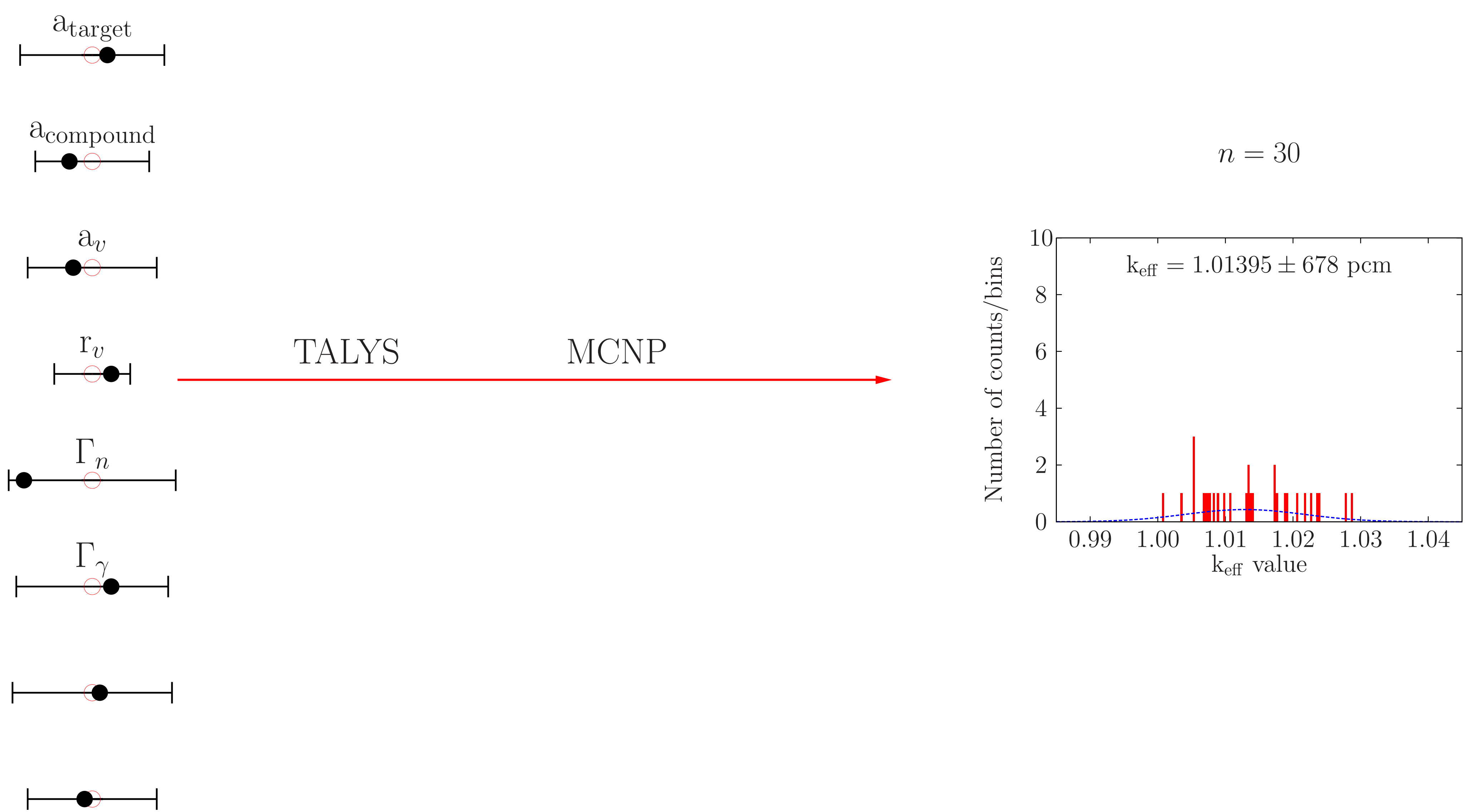

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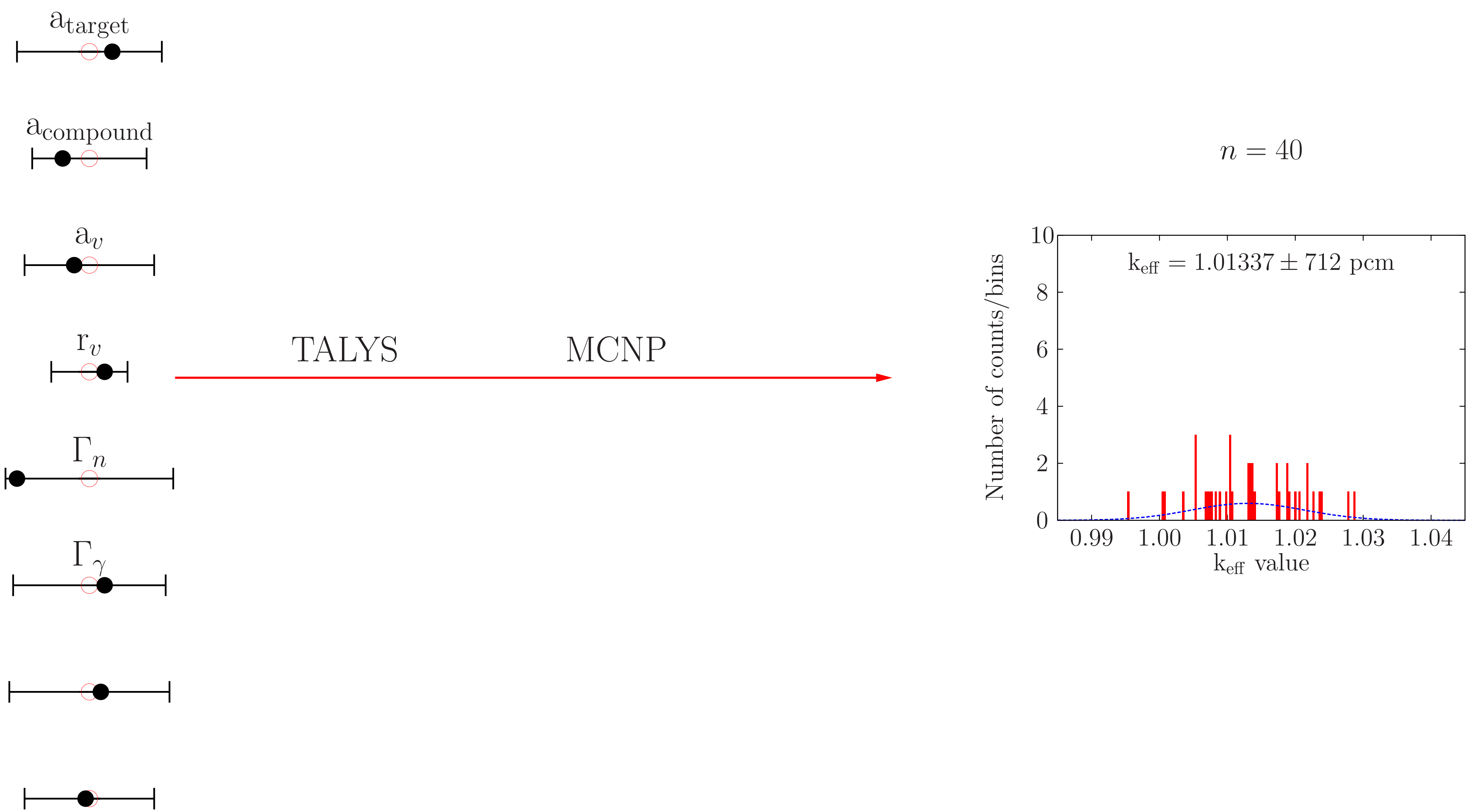

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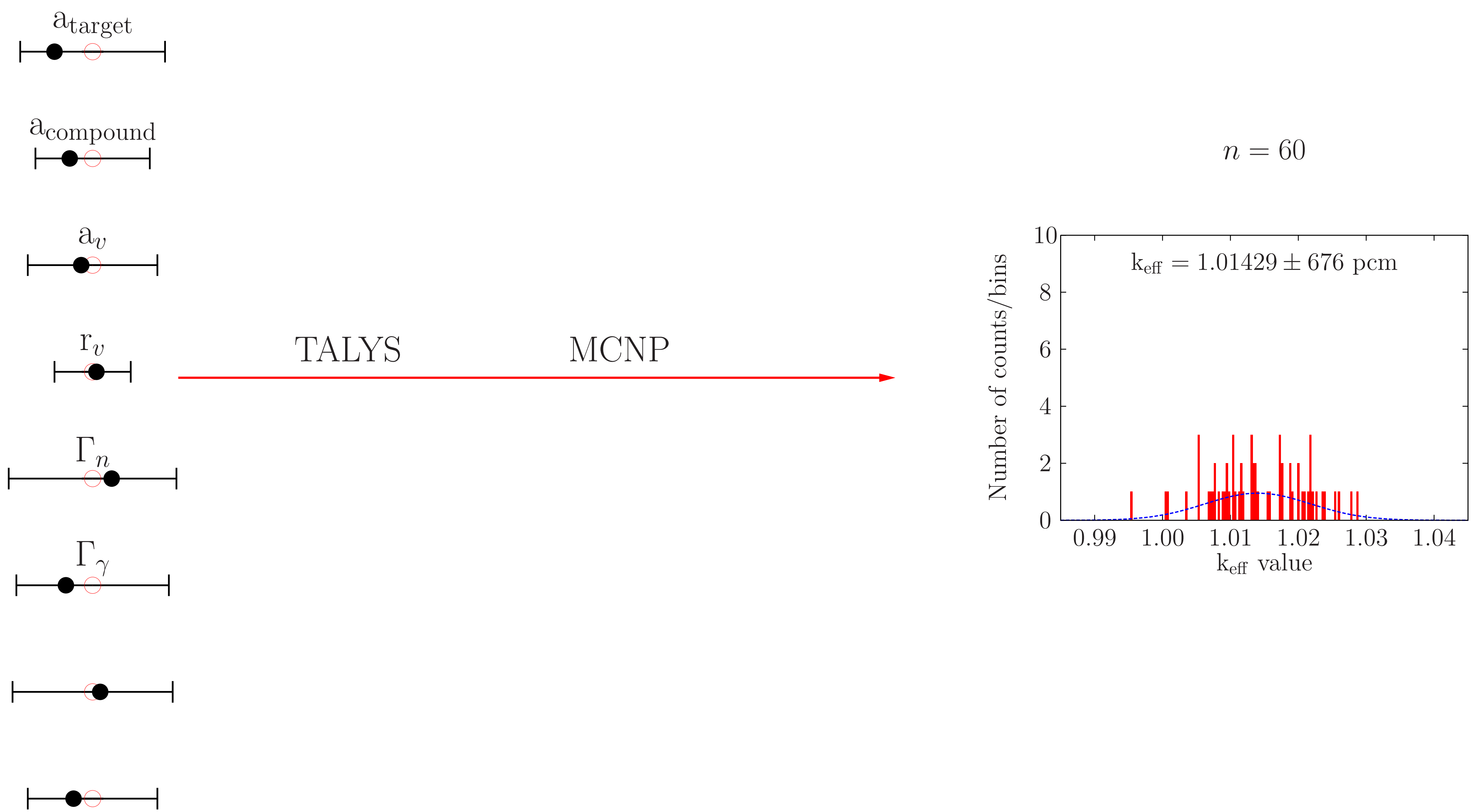

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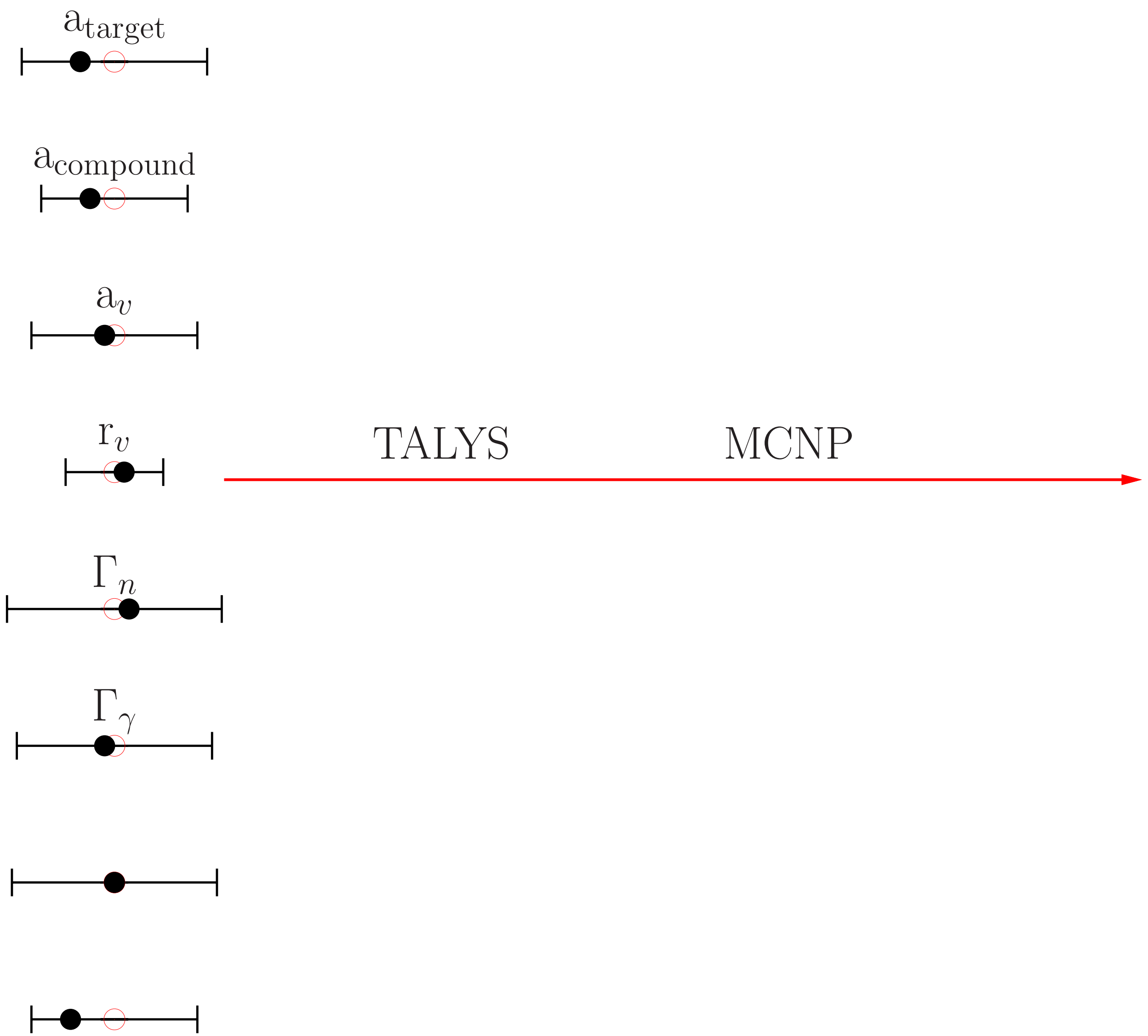
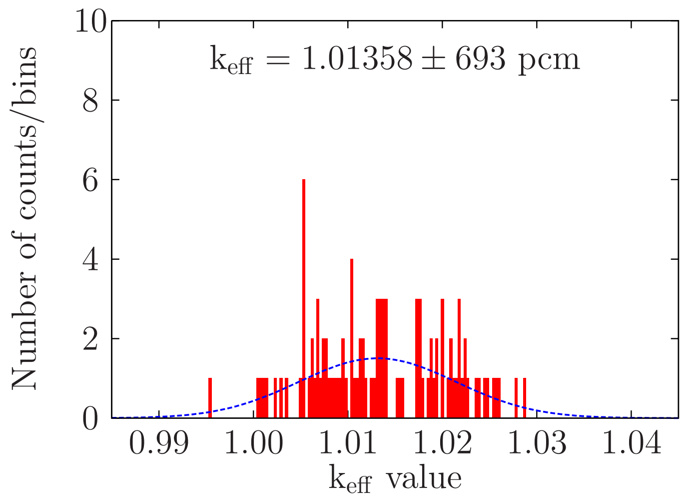


$n = 100$



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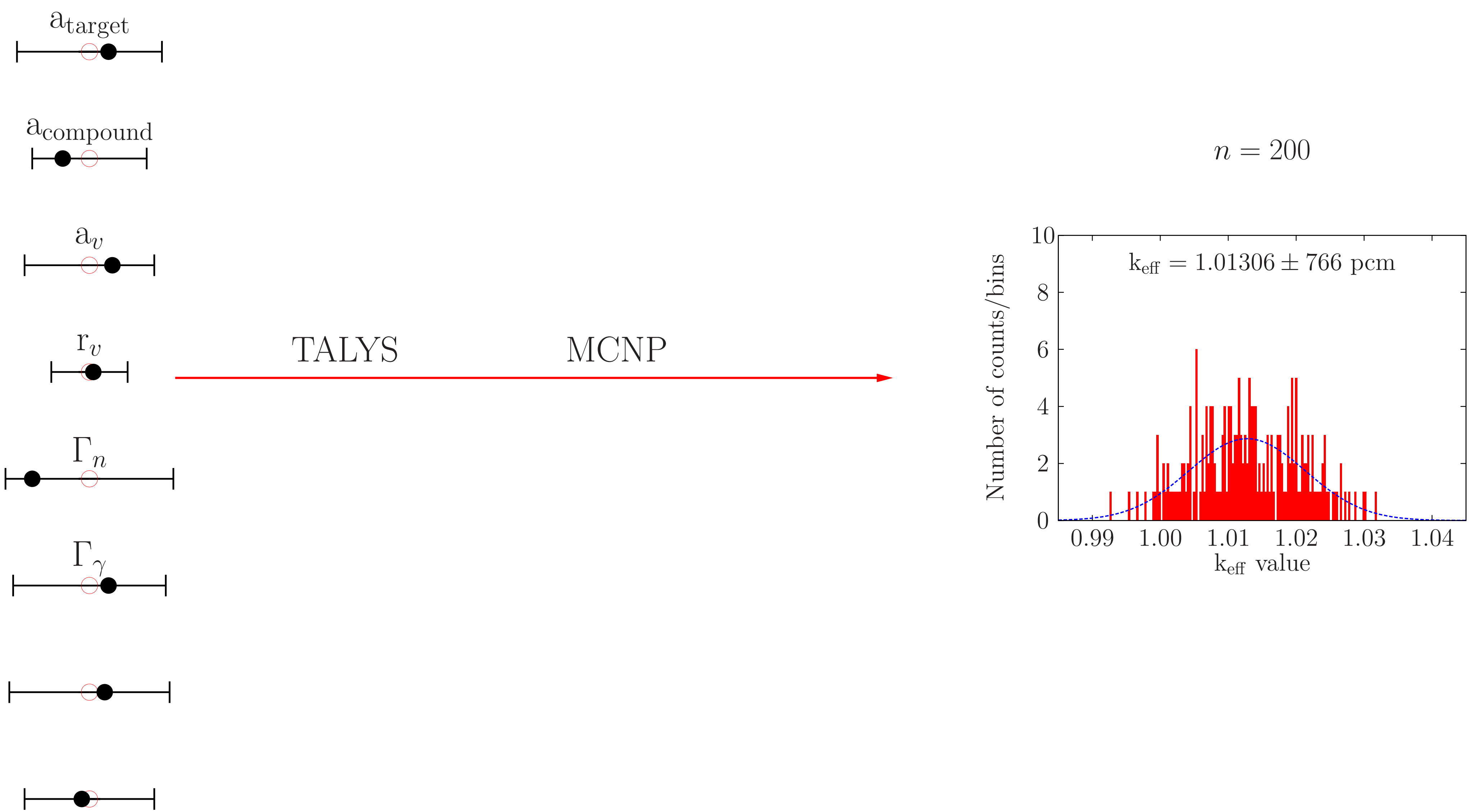

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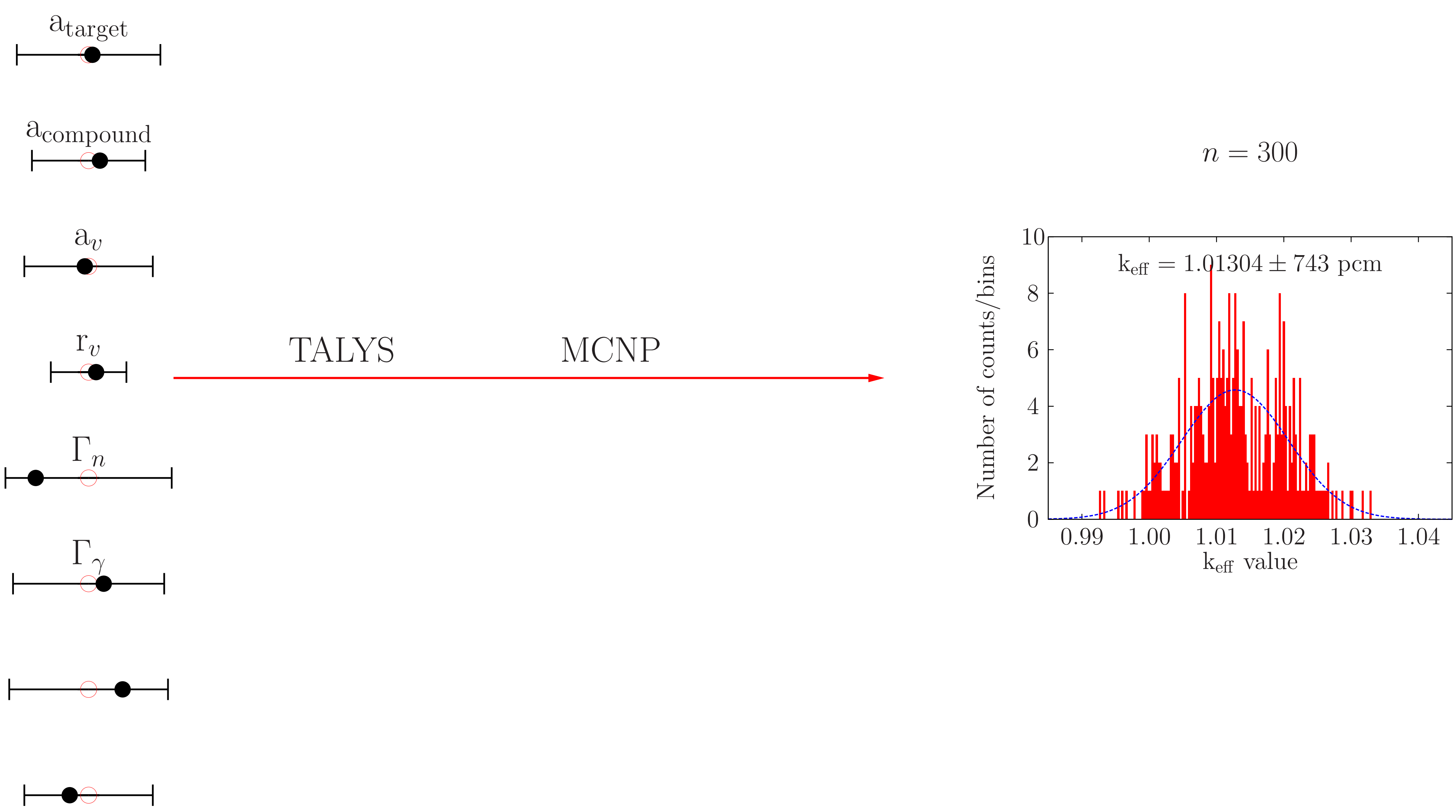

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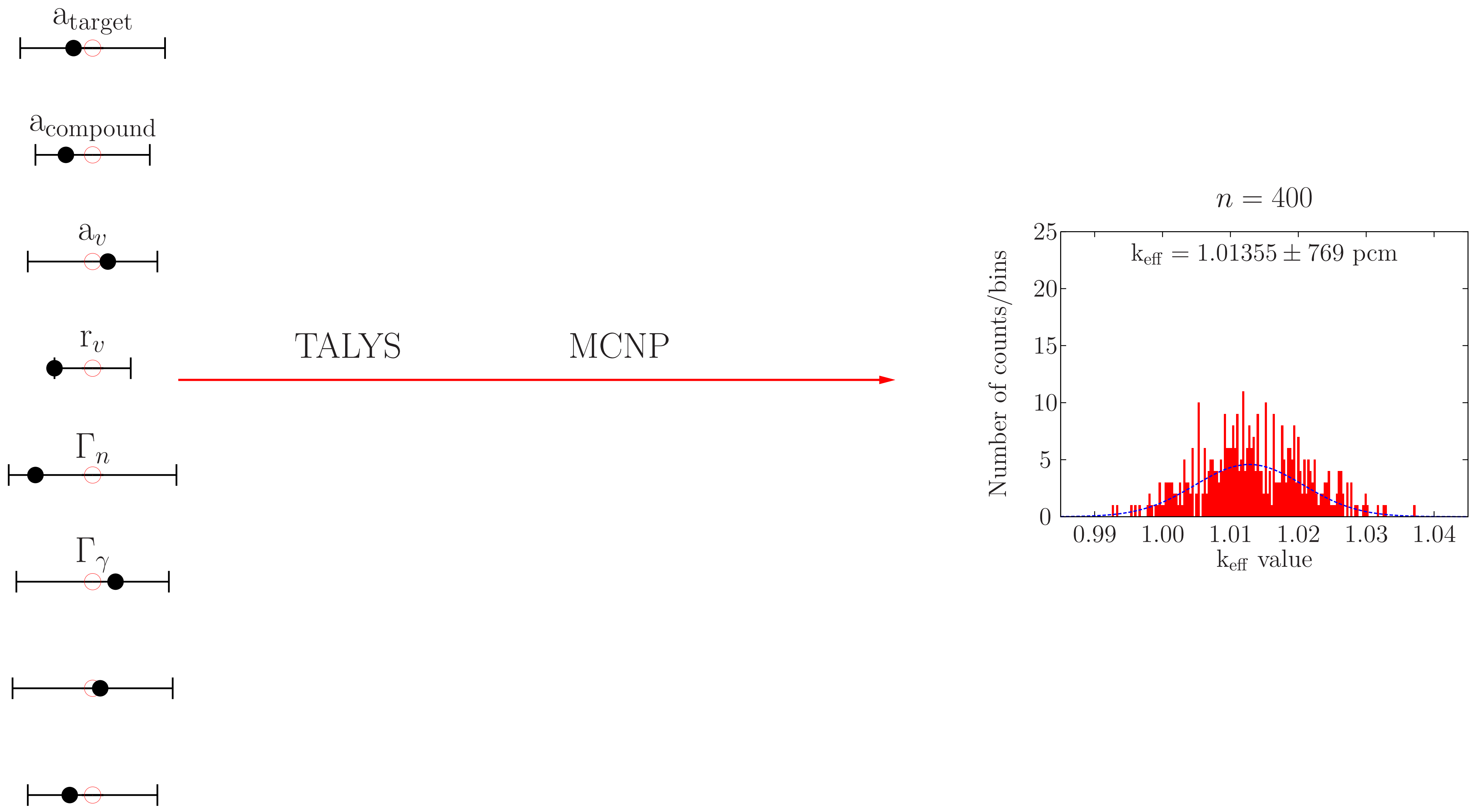

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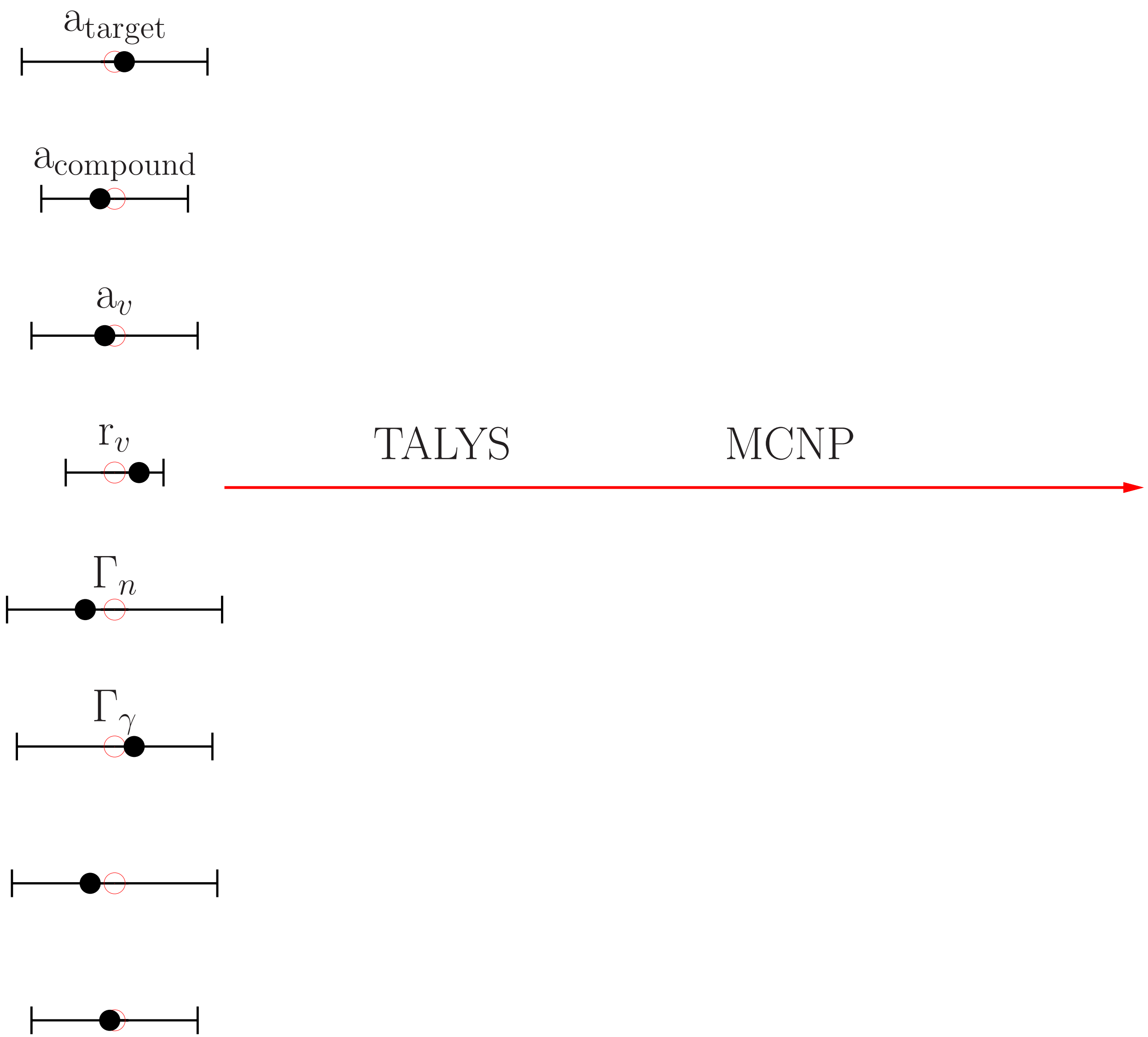

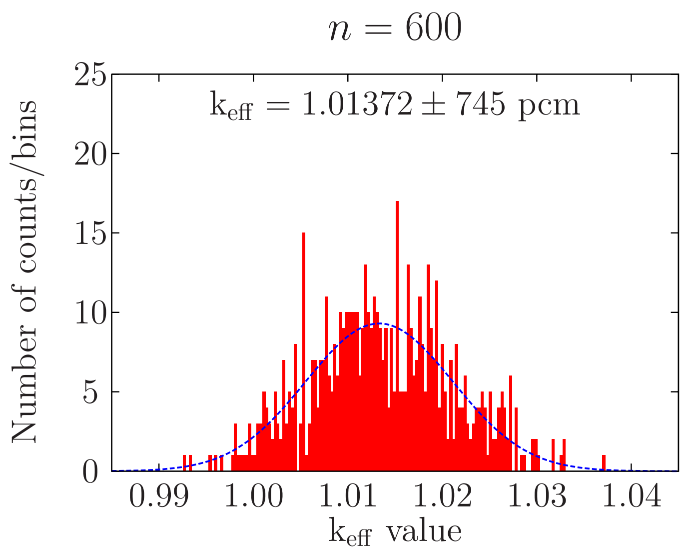

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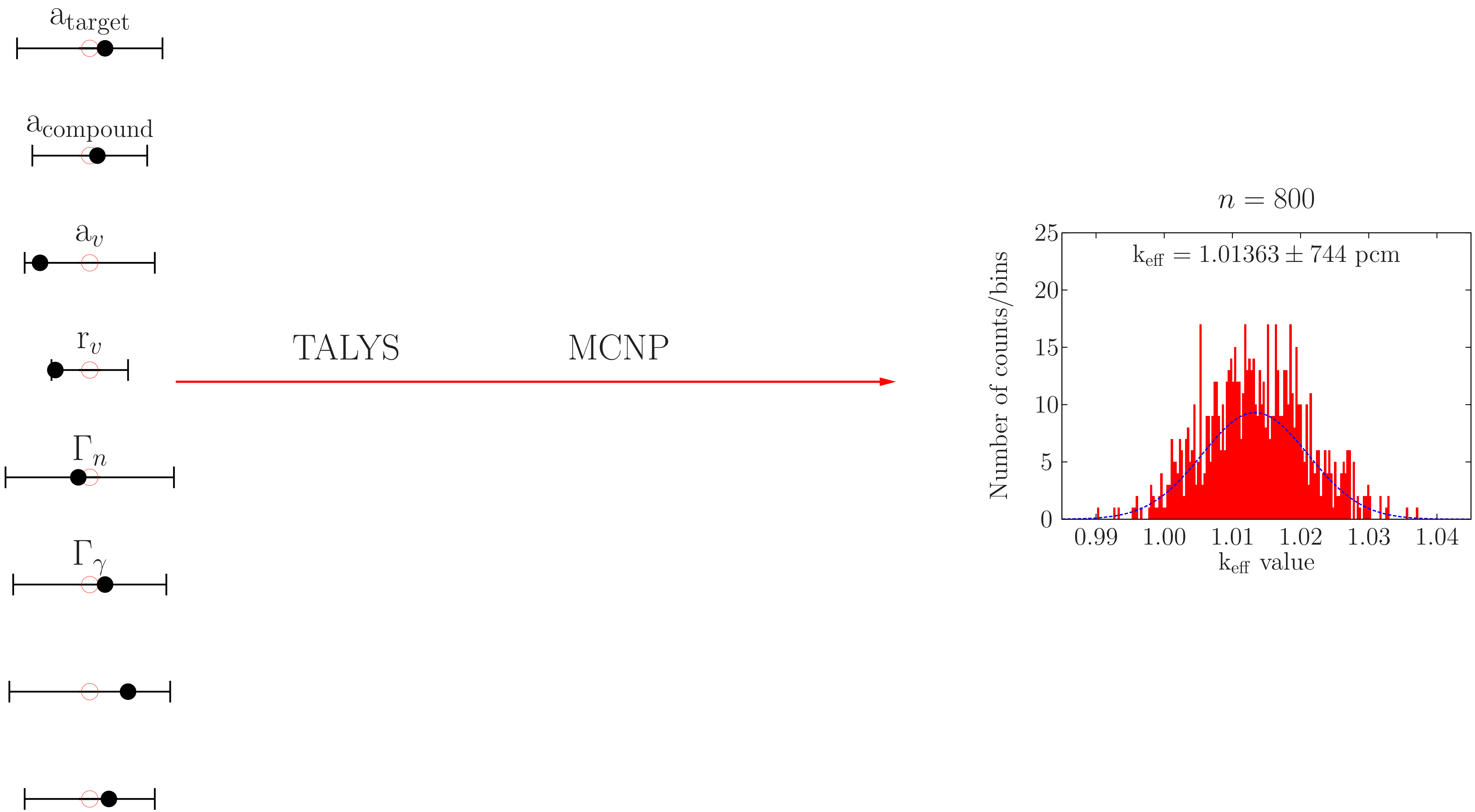

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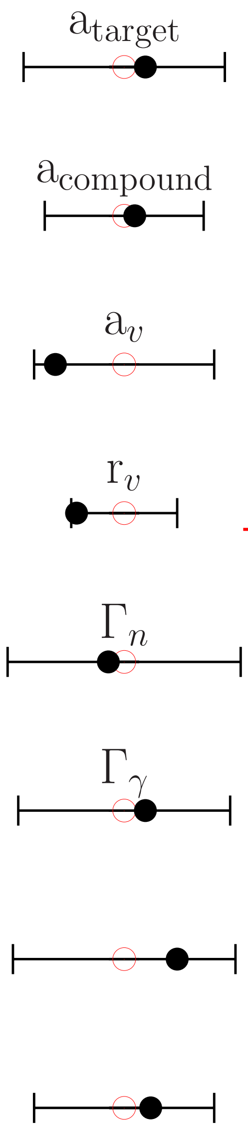

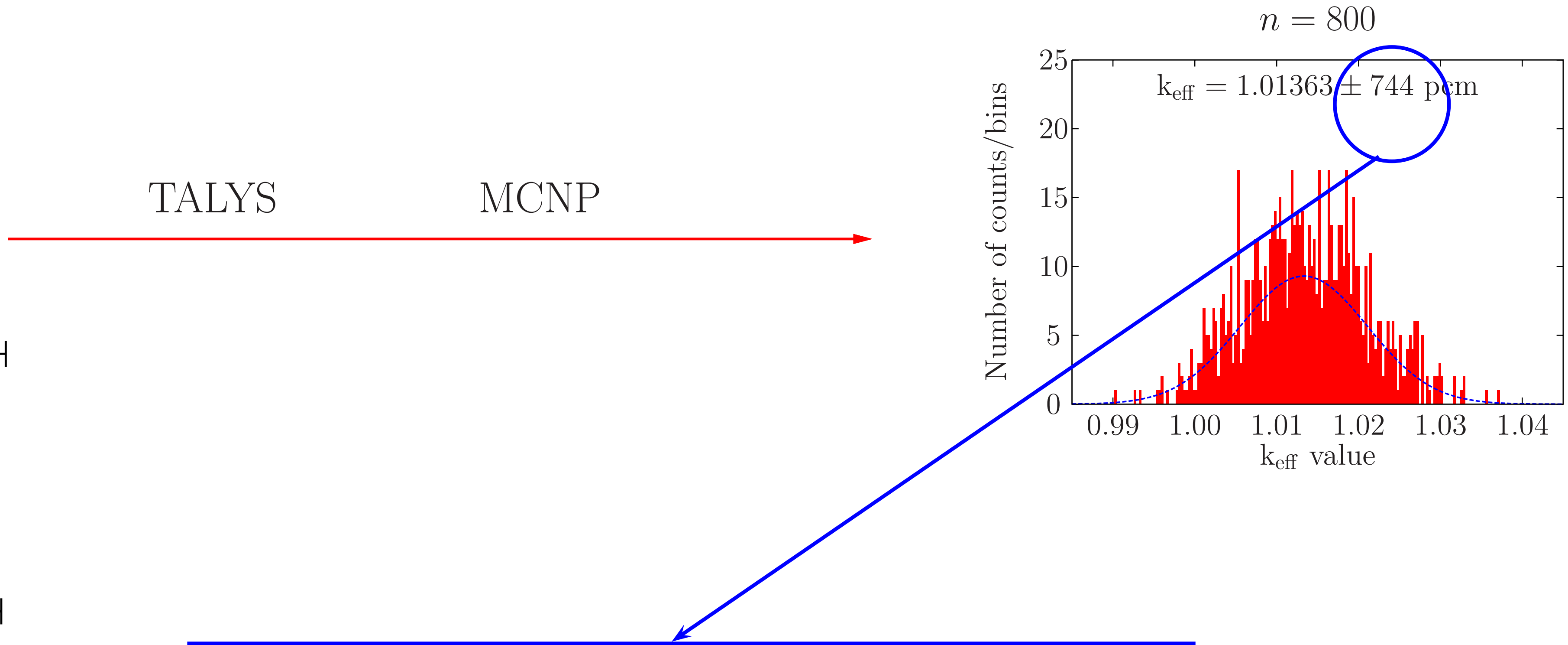

Statistical uncertainty $\simeq$ 68 pcm

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

Considered data in TMC (or fast TMC)

Several hundreds of random ENDF files for transport + depletion

- 3 Major actinides: ^{235}U, ^{238}U, ^{239}Pu,
- Light elements: lighter than oxygen,
- Thermal scattering data: H in H_2O, D in D_2O, C in Carbon,
- All Fission yields (e.g. ^{234,235,236,238}U, ^{239,240,241}Pu, ^{237}Np, ^{241,243}Am, ^{243,244}Cm),
- All Minor actinides (e.g. ^{234,236,237}U, ^{237}Np, ^{238,240,241,242}Pu, Am, Cm),
- All fission products (e.g. from Ge to Er), and decay data,

(fast) TMC can be applied to any input data, propagating uncertainties to any outputs

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- All fission products (e.g. from Ge to Er), and decay data,

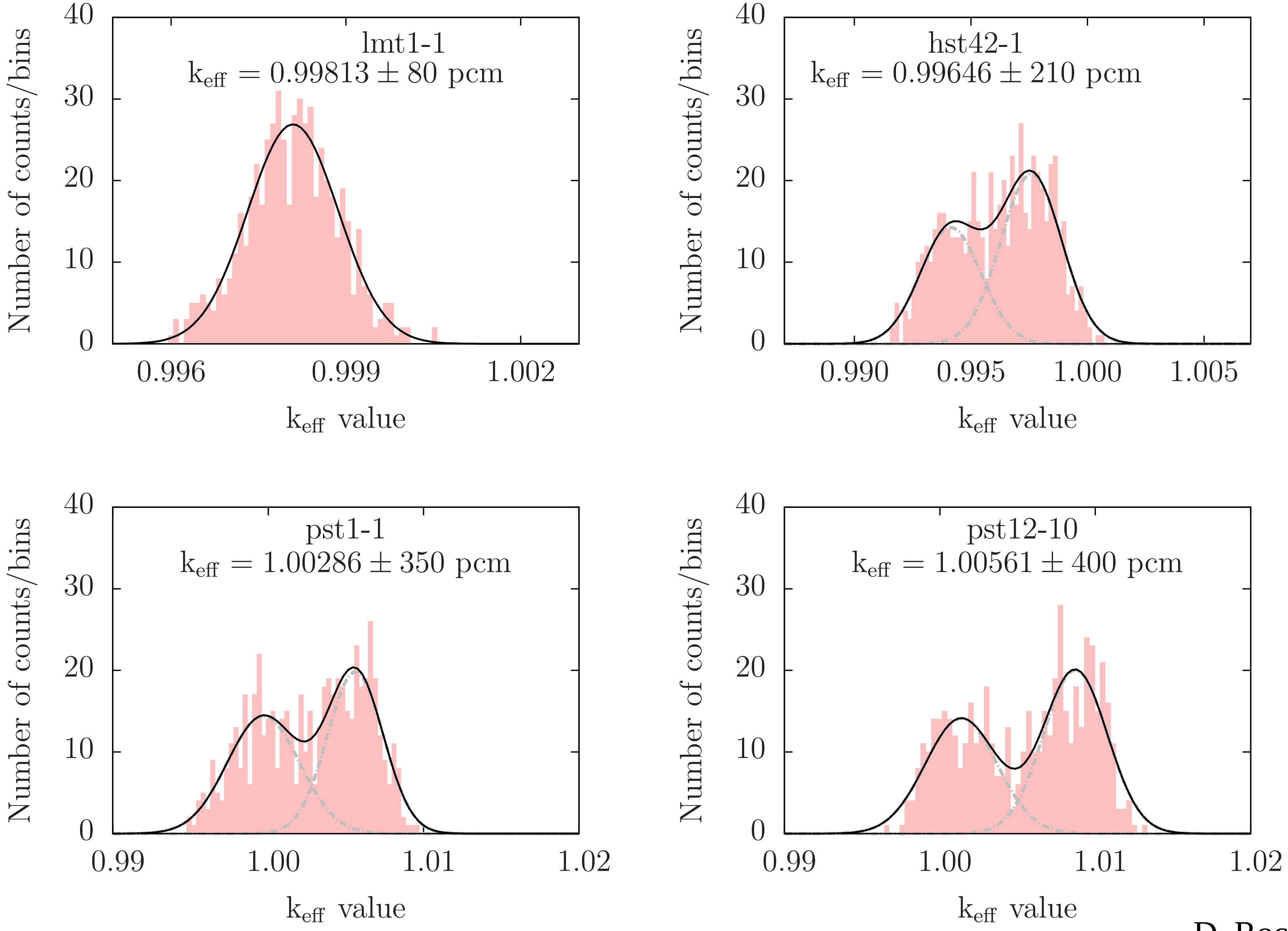
(fast) TMC can be applied to any input data, propagating uncertainties to any outputs

TMC was already applied to

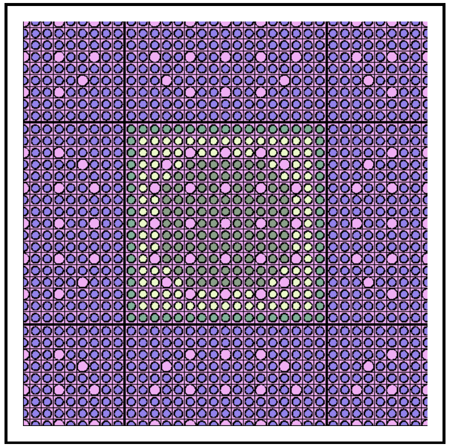
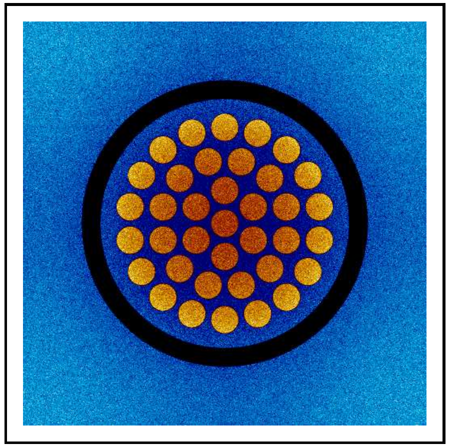
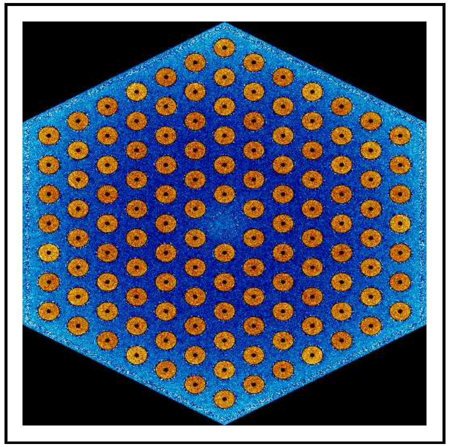
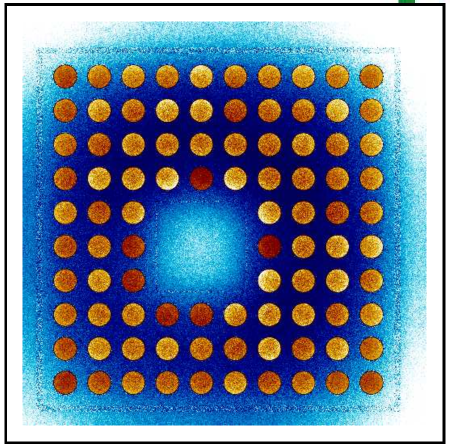
- criticality-safety, shielding, pincell/assembly burn-up, full core, activation,
- PWR, BWR, Gen-IV systems,
- UO_2, MOX fuels,
- MCNP, SERPENT, FISPACT, DRAGON, PANTHER, RELAP-5

Application: thermal scattering for H in H_2O or $S(\alpha,\beta)$ tables (with MCNP)

Random parameters of the $S(\alpha,\beta)$ for inelastic scattering

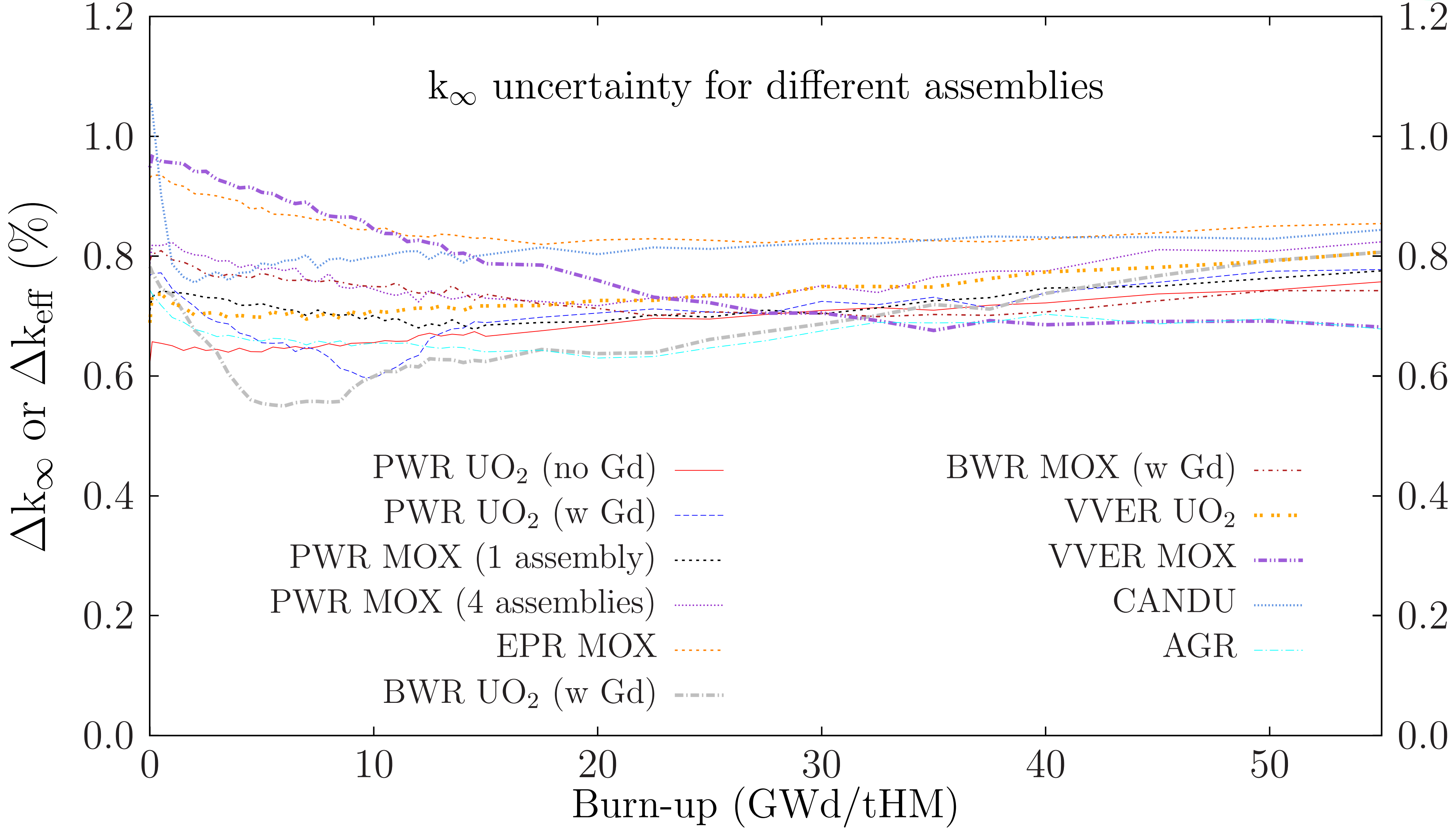


Systematical study on UO_2/MOX assembly uncertainties

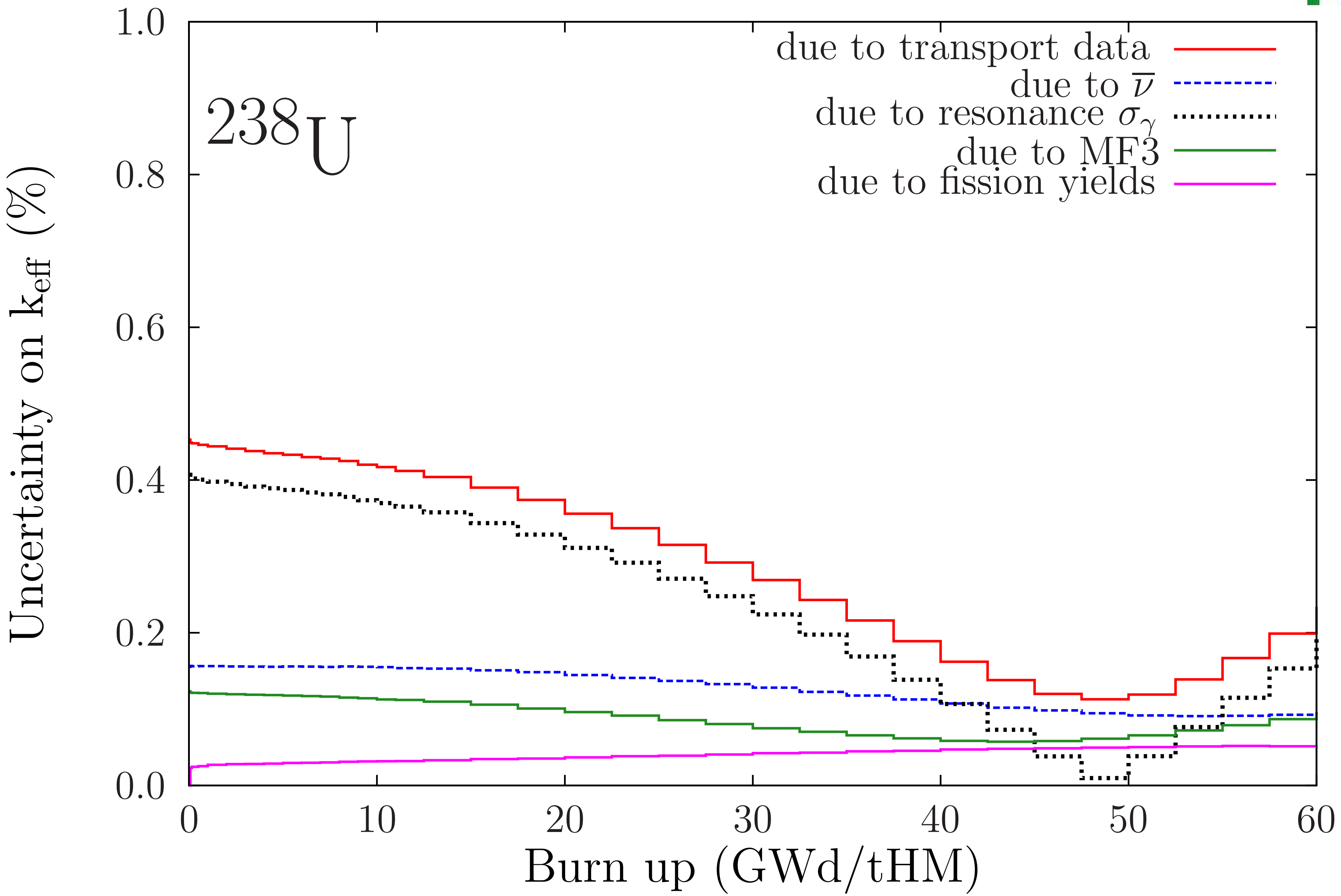





- Different UO_2/MOX assemblies (PWR, BWR, VVER, AGR, CANDU, fast systems),
- Burn-up calculated with SERPENT,
- All major nuclear data taken into account.
- $\Longrightarrow$ systematical study on k_{eff}, inventory, heat...

Comparison of Δk_∞ for assemblies and full core (SERPENT)



TMC applied to PWR assembly burn-up calculations with DRAGON



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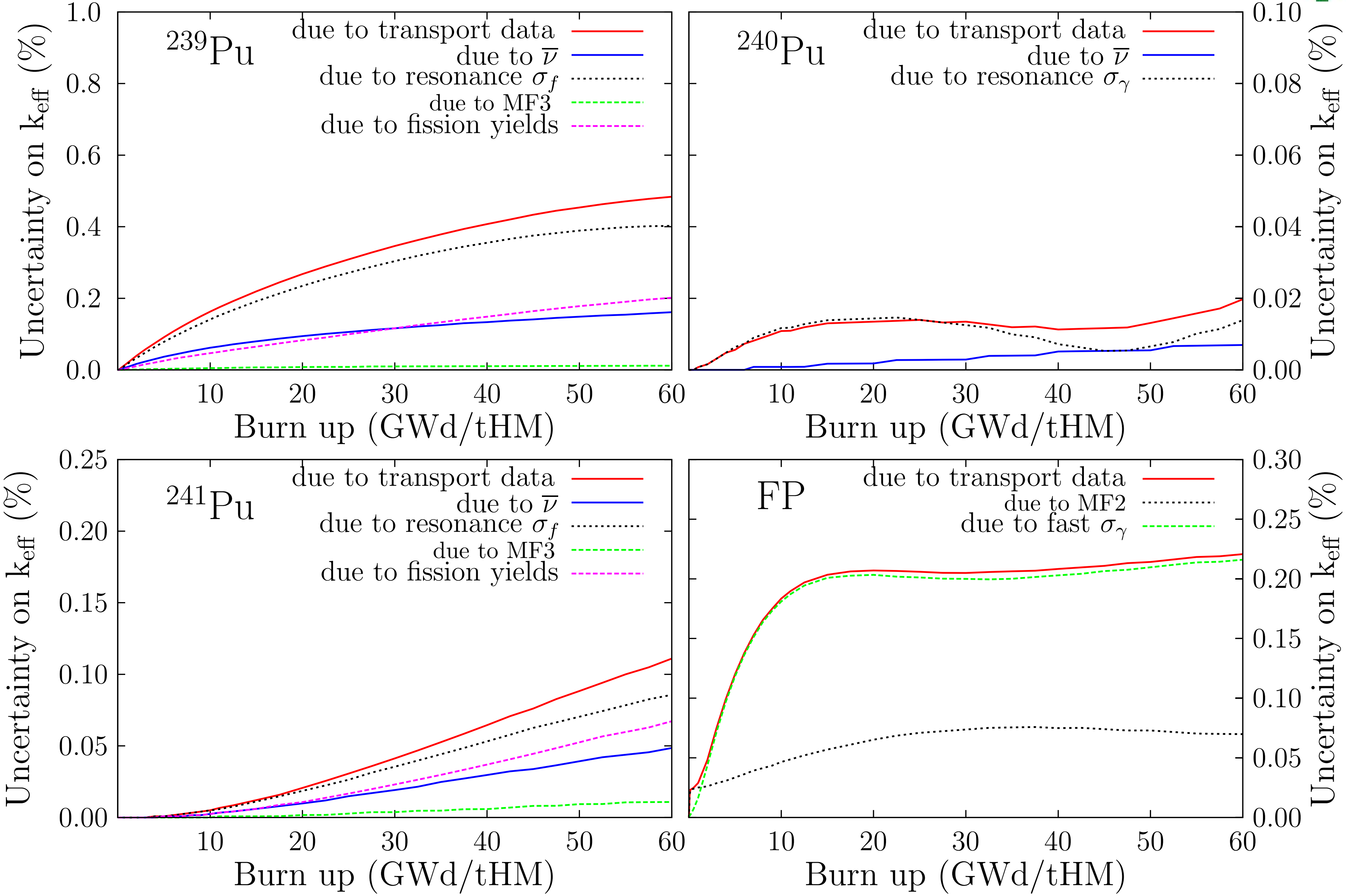
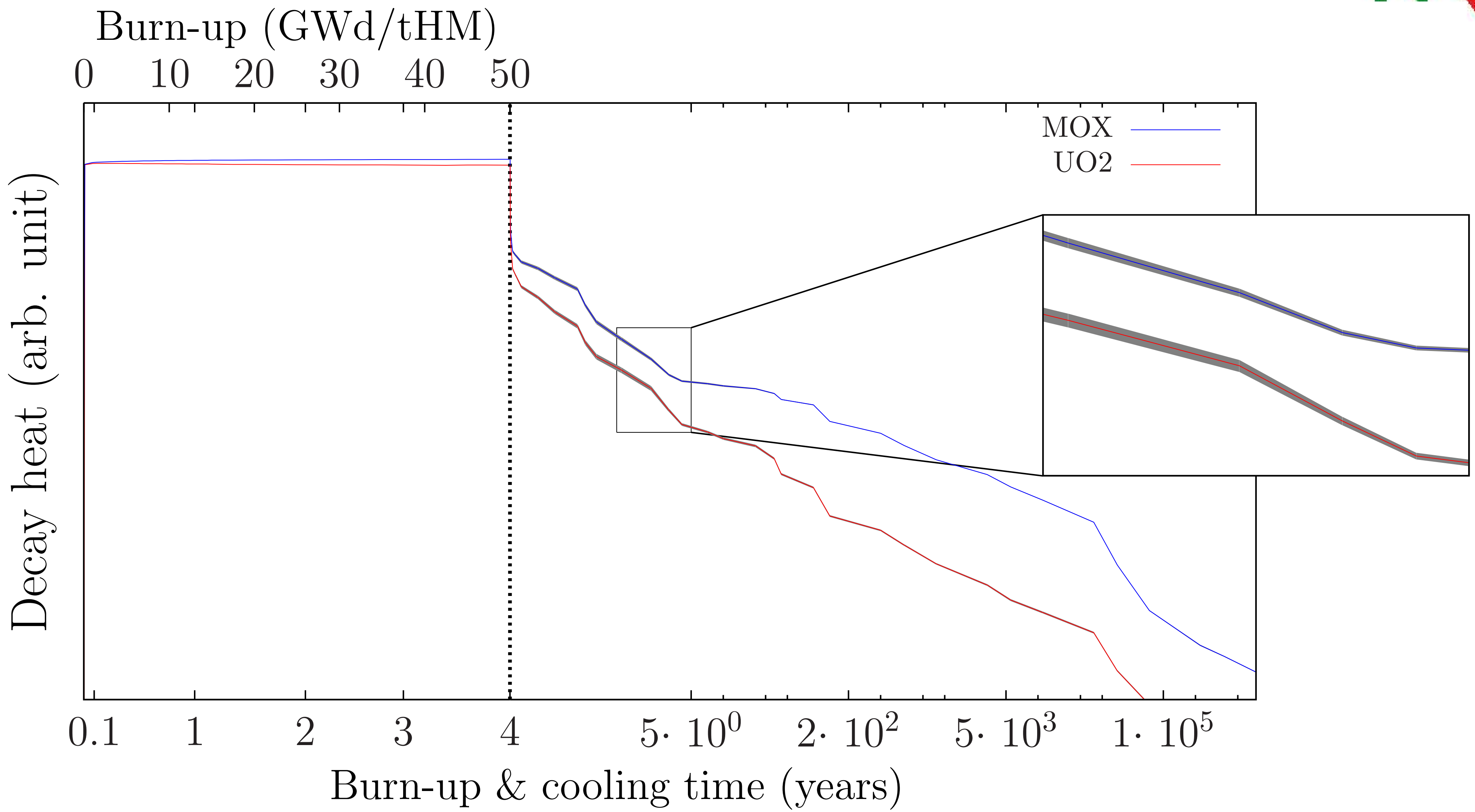
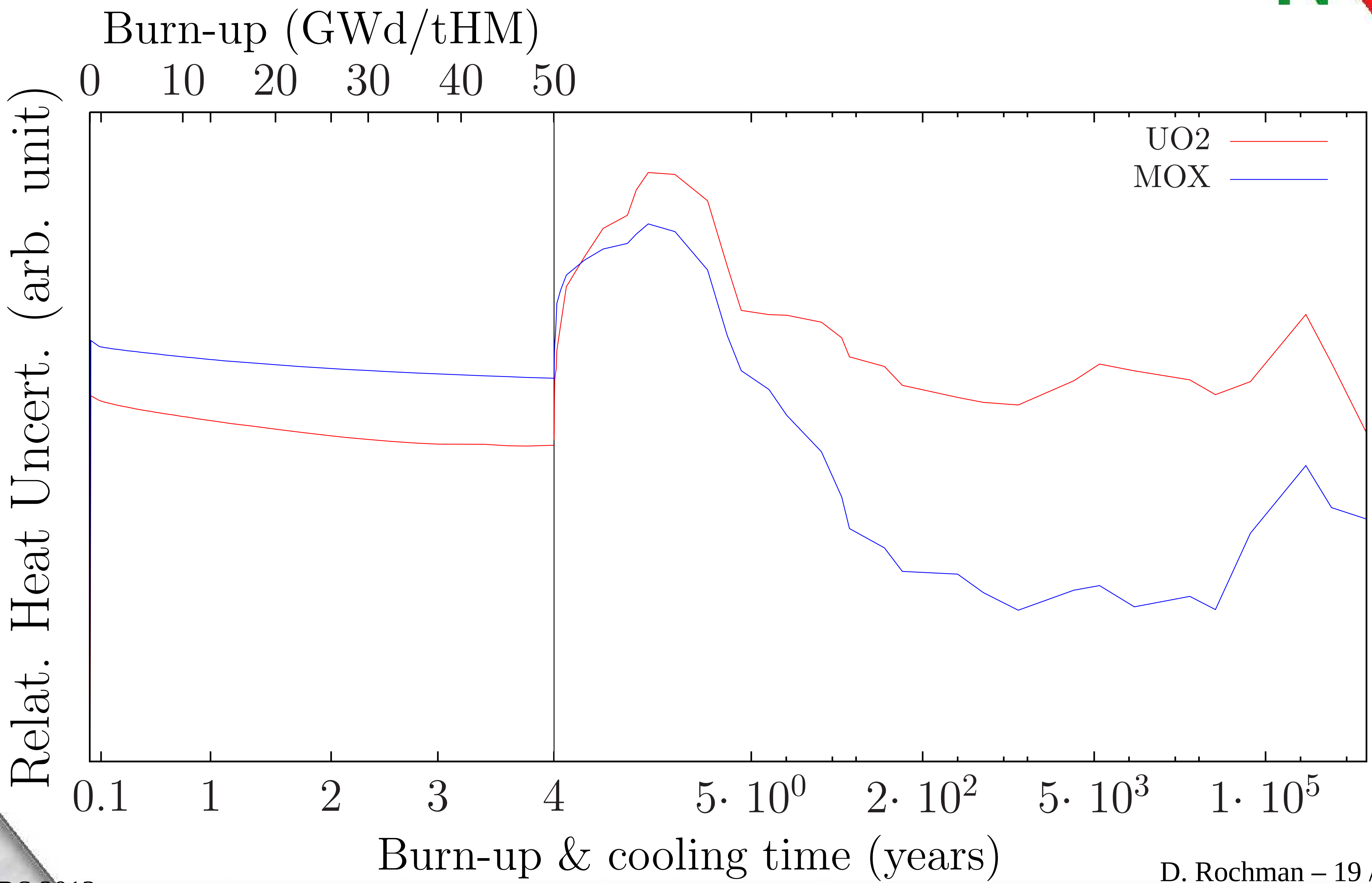


TMC applied for burn-up calculations: decay heat



TMC applied for burn-up calculations: decay heat uncertainties



Effect of H in H_2O for a full core PWR (courtesy of O. Cabellos, UPM, Spain)

Method: TMC applied to COBAYA (3D multigroup core calculations) + SIMULA (coupled neutronic-thermohydraulics 3D core calculations)

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III.2 PWR problem description

PWR (WESTINGHOUSE), 3 loops , 157 FA, power 2775. MWth

¼ CORE

	1	2	3	4	5	6	7	8
1	1	13	4	**21**	6	**21**	16	14
2	13	11	15	2	16	6	**20**	7
3	4	15	3	**21**	8	**22**	**19**	
4	**21**	2	**21**	9	18	**20**	5	
5	6	16	8	18	12	17		
6	**21**	6	**22**	**20**	17			
7	16	**20**	**19**	10				
8	14	7						

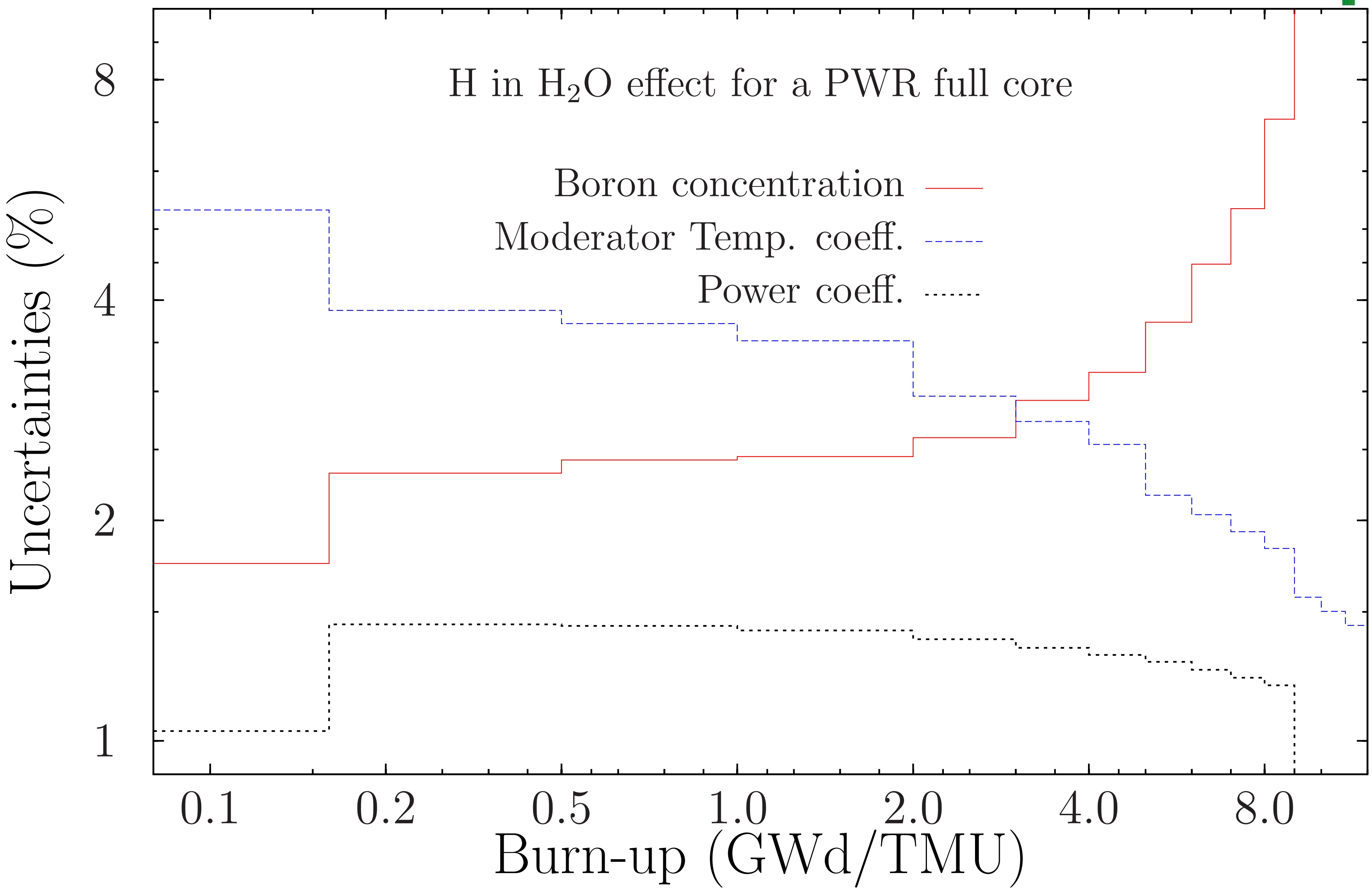
AVE. BURNUP PER FUEL ASSEMBLY

	1	2	3	4	5	6	7	8
1	18.137	11.662	27.397	0.000	30.867	0.000	14.984	11.662
2	11.662	16.188	13.130	28.902	12.155	28.866	0.000	30.191
3	27.397	13.130	27.572	0.000	22.778	0.000	0.000	
4	0.000	28.902	0.000	30.755	15.236	0.000	30.124	
5	30.867	12.155	22.778	15.236	13.123	14.882		
6	0.000	28.866	0.000	0.000	14.882			
7	14.984	0.000	0.000	30.503				
8	11.662	30.191						

FUEL	TYPE	w/o(%)	WABAS
1	OFA	2.10	0
2	OFA	3.10	0
3	OFA	3.24	0
4	OFA	3.24	0
5	OFA	3.24	0
6	OFA	3.24	0
7	OFA	3.24	0
8	OFA	3.24	0
9	OFA	3.24	0
10	OFA	3.24	0
11	OFA	3.24	0
12	AEF	3.60	0
13	AEF	3.60	0
14	AEF	3.60	0
15	AEF	3.60	0
16	AEF	3.60	0
17	AEF	3.60	0
18	AEF	3.60	0
19	AEF	3.60	0
20	AEF	3.60	4
21	AEF	3.60	8
22	AEF	3.60	12

UAM7 – Paris (France), April 10-12, 2013 20

Effect of H in H_2O for a full core PWR (courtesy of O. Cabellos, UPM, Spain)



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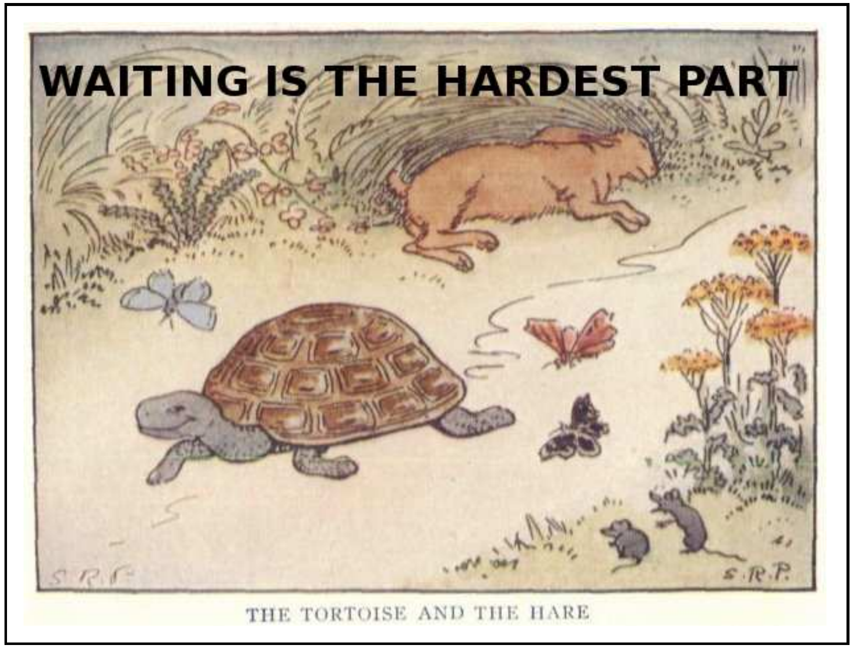

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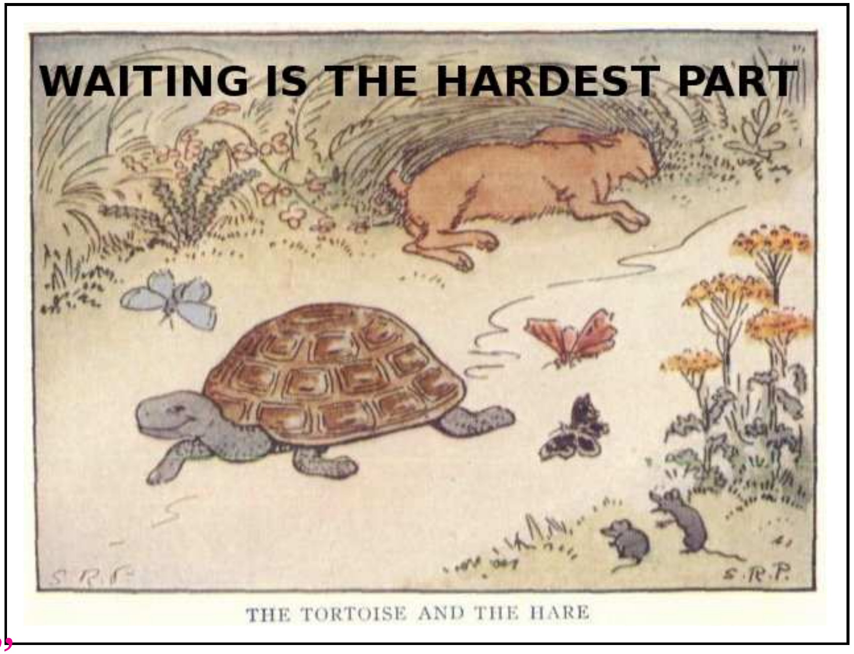

There is a solution with Monte Carlo codes:
(in fact 2 solutions)

- fast GRS method,
- and fast TMC.

"Efficient use of Monte Carlo: uncertainty propagation",
D. Rochman, W. Zwermann et al., submitted to NSE, May 2013.

2012: fast GRS method

First presented in PHYSOR-2012 by W. Zwermann *et al.*. It takes advantage of conditional expectations:

> If two output variables $k^{(1)}$ and $k^{(2)}$ are identically distributed and conditionally independent given the vector of nuclear data input then
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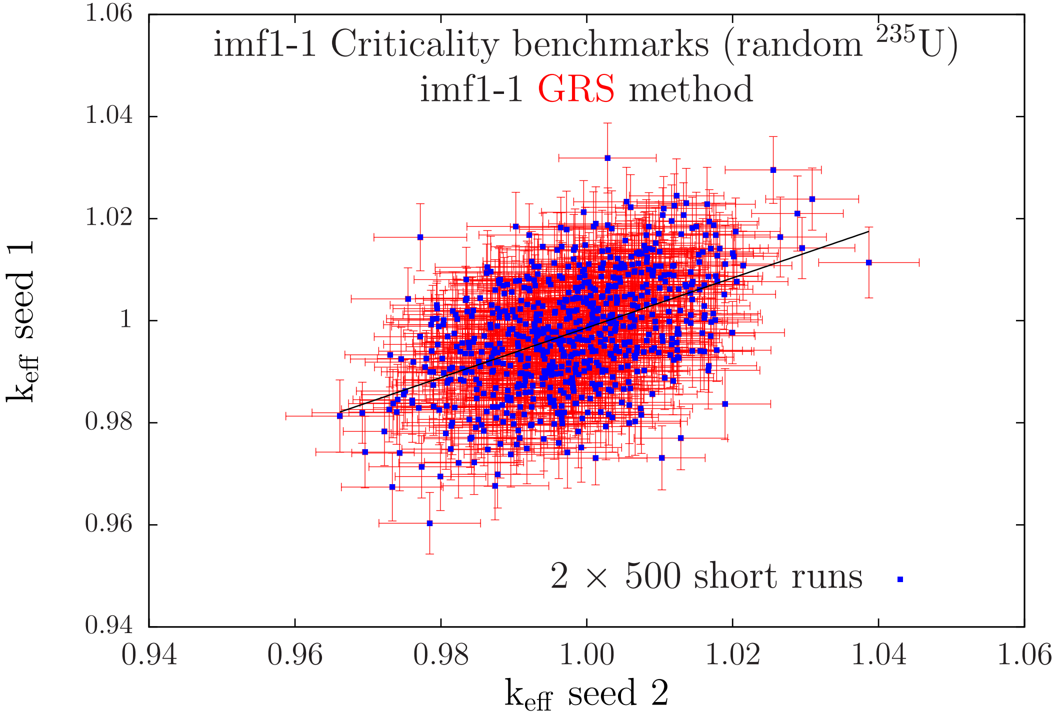
$$\sigma_{\text{nuclear data}} = \sqrt{\text{cov}(k^{(1)}, k^{(2)})}$$

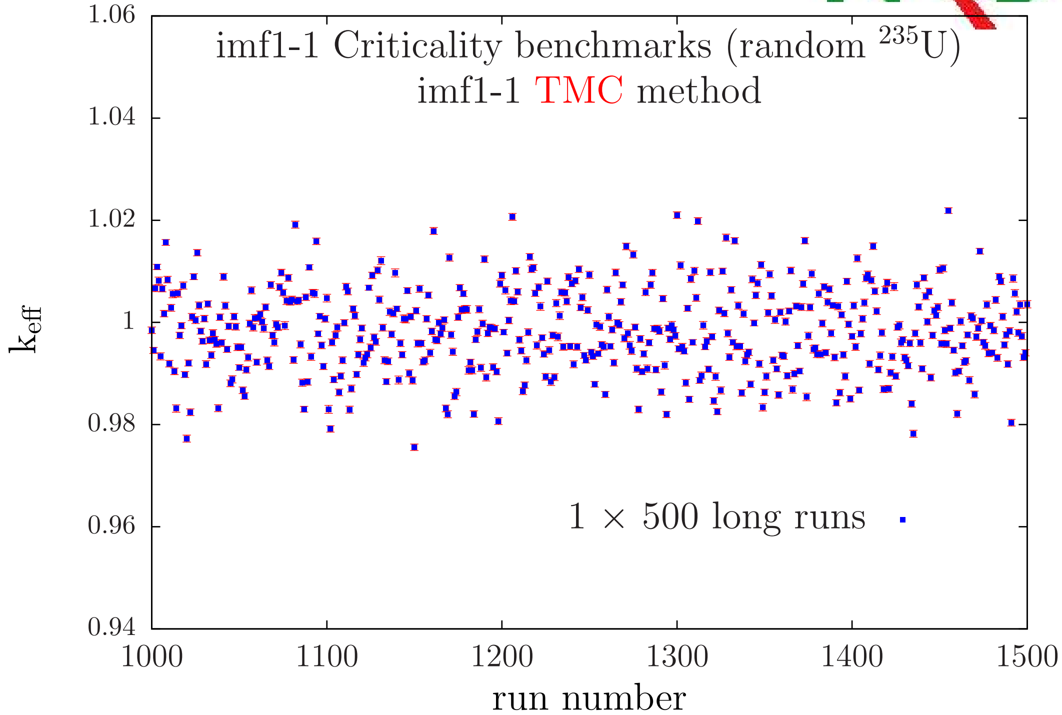
In practice:

1. perform $i = 1..500$ MCNP short calculations with random nuclear data and a fixed seed $s_1 \Longrightarrow k_{\text{eff}}^{(1)}(i)$
2. repeat for $j = 1..500$, same random nuclear data but fixed seed $s_2 \Longrightarrow k_{\text{eff}}^{(2)}(j)$

There is no necessity to have small $\sigma_{\text{statistics}}$!!
each run can be (very) short

fast GRS method





$$\sigma_{\text{nucl.data}} = \sqrt{\text{cov}(\vec{k_1}, \vec{k_2})} = \sqrt{\text{corr}(\vec{k_1}, \vec{k_2}) \times \sigma_1 \sigma_2}$$
$$= \sqrt{0.48 \times 0.0110 \times 0.0112}$$
$$= 770 \text{ pcm}$$

$$\sigma_{\text{nucl.data}} = \sqrt{\sigma_1^2 - \sigma_{\text{stat}}^2}$$
$$= \sqrt{0.0805^2 - 0.00067^2}$$
$$= 802 \text{ pcm}$$

2 × 500 ”*short*” runs ∼ 2 × ”*long*” run in time

2013: fast TMC method...

If a single calculation takes m histories (σ_{stat} small enough), then repeat it n times with m/n histories, random nuclear data and random seeds.

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

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⋮		⋮			⋮
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n runs		$\sigma(\overline{k}) \sim \sigma_{stat}$		T sec.	

$$\begin{cases} \sigma^2_{total} = \frac{1}{n-1}\sum_{i=1}^{n}\left(k_i - \overline{k}\right)^2 \\ \sigma^2_{statistics} = \frac{1}{n}\sum_{i=1}^{n}\sigma^2_i \end{cases}$$

The fast methods

- ☺ as fast as S/U methods (1-2 $\times$ longer than 1 single calculation),
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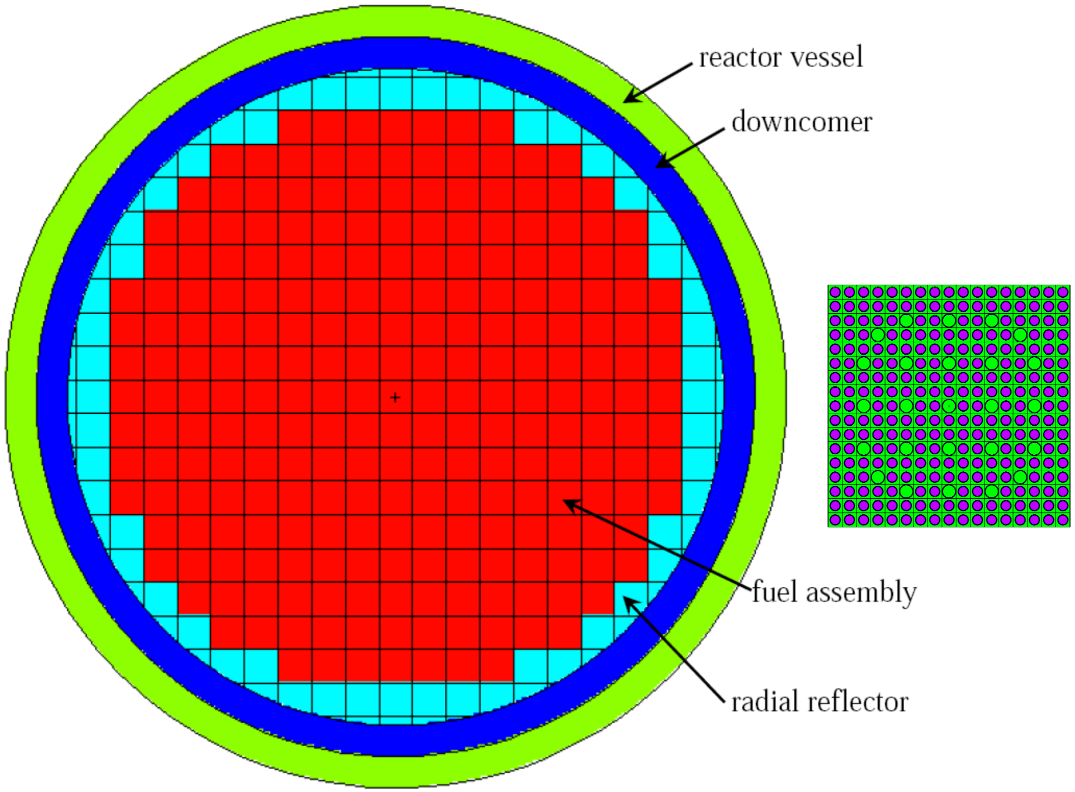
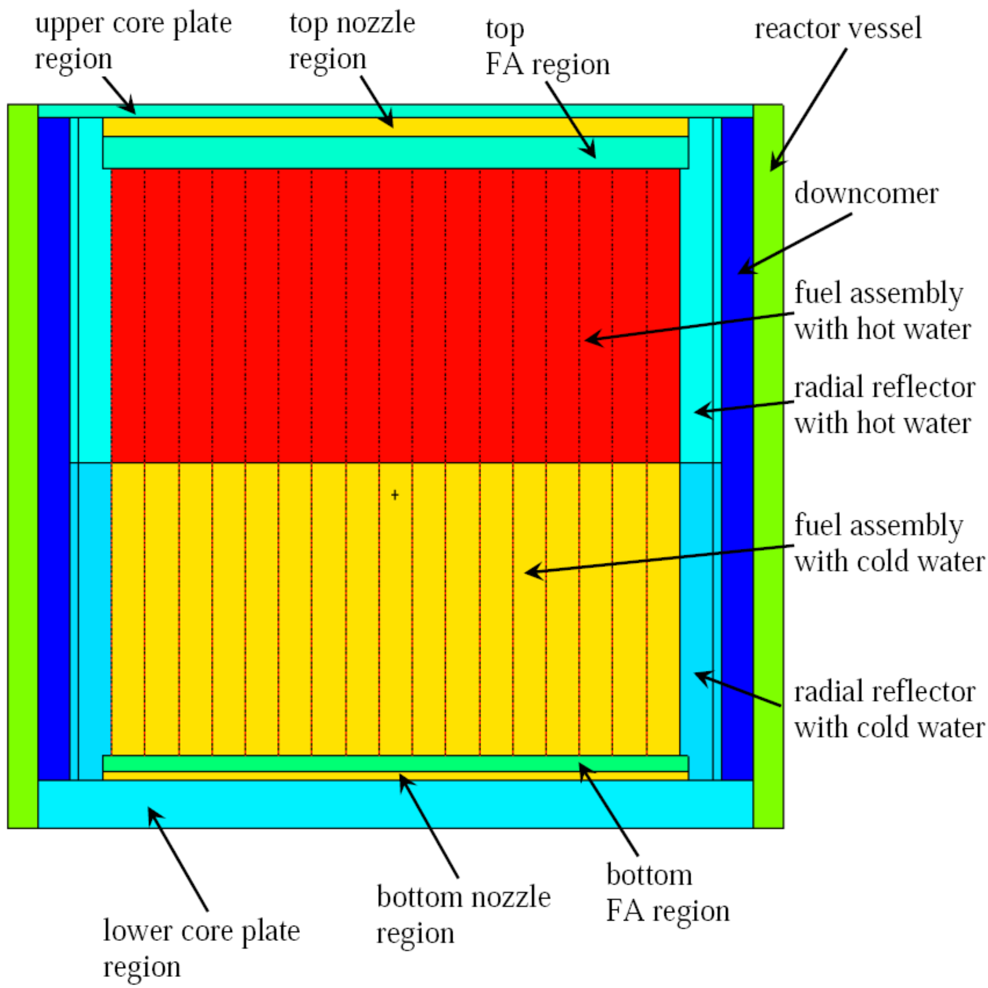
- ☺ Example: the Martin-Hoogenboom benchmark

MCNP6 model: 241 fuel assemblies, with 264 fuel pins each





Fast TMC & GRS methods on a full core

- $357 \times 357 \times 100$ regions ($1.26 \times 1.26 \times 3.66$ cm^3): 6.4 million cells for generated power (f7)
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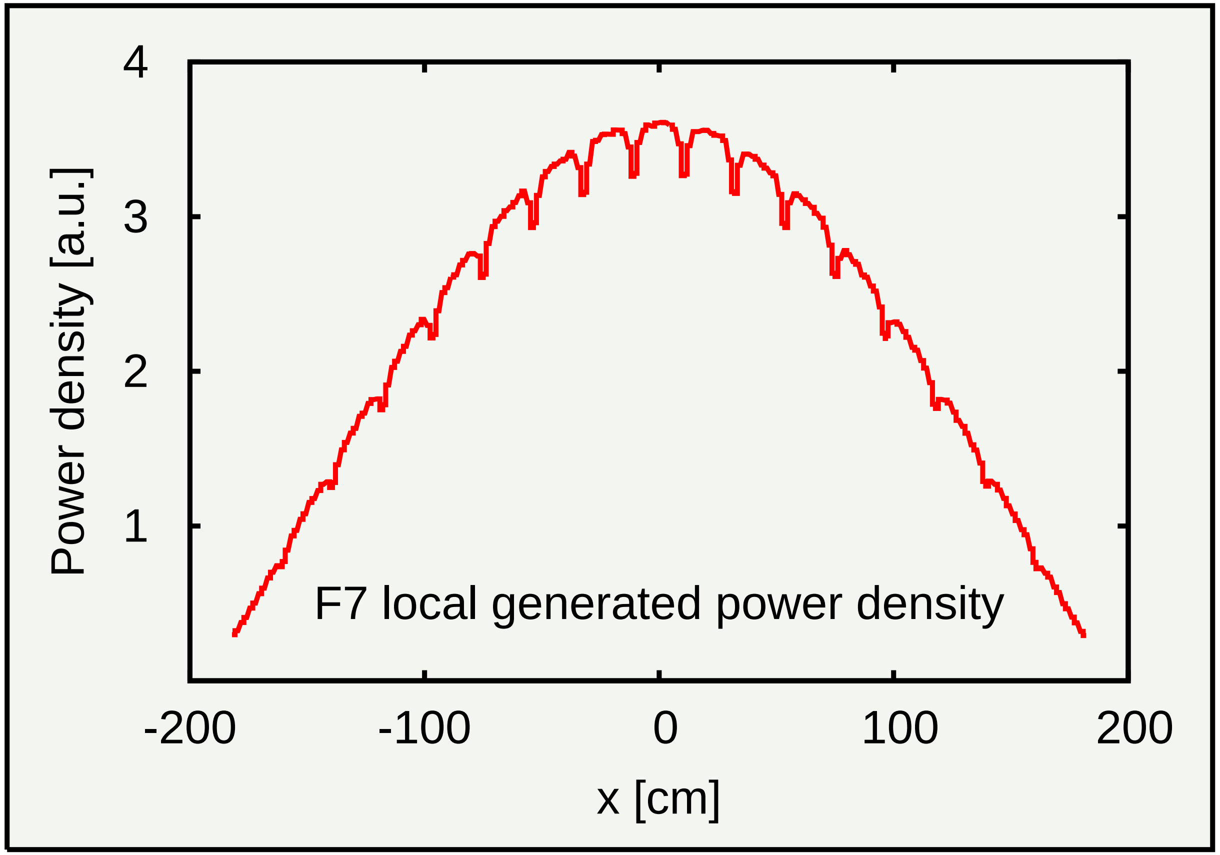
- ➼ Uncertainty on local pin power due to ^{235}U, ^{238}U, ^{239}Pu and H in H_2O thermal scattering in each cell ?



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(1) Source convergence

- For both methods, a first calculation is run with fixed nuclear data to obtain a reasonably converged fission source.
- All subsequent short simulations start with this fission source:
  - each with 10 inactive cycles and 90 active cycles of 4×10^6 histories, and random nuclear data,
  - source convergence tested with the MCNP6 built-in indicator (fission source entropy).
  - 362 short runs out of 508 were then accepted for fast TMC.
  - 2×122 short runs out of 2×328 were then accepted for fast GRS.

Fast TMC & GRS methods on a full core

(2) Statistical uncertainty estimation

- In MCNP eigenvalue calculation, σ_{stat} is usually underestimated.
- An independent estimation of σ_{stat} is therefore necessary for fast TMC,
- From the 508 short runs, the first 389 were repeated with fixed nuclear data,
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Fast TMC & GRS methods on a full core

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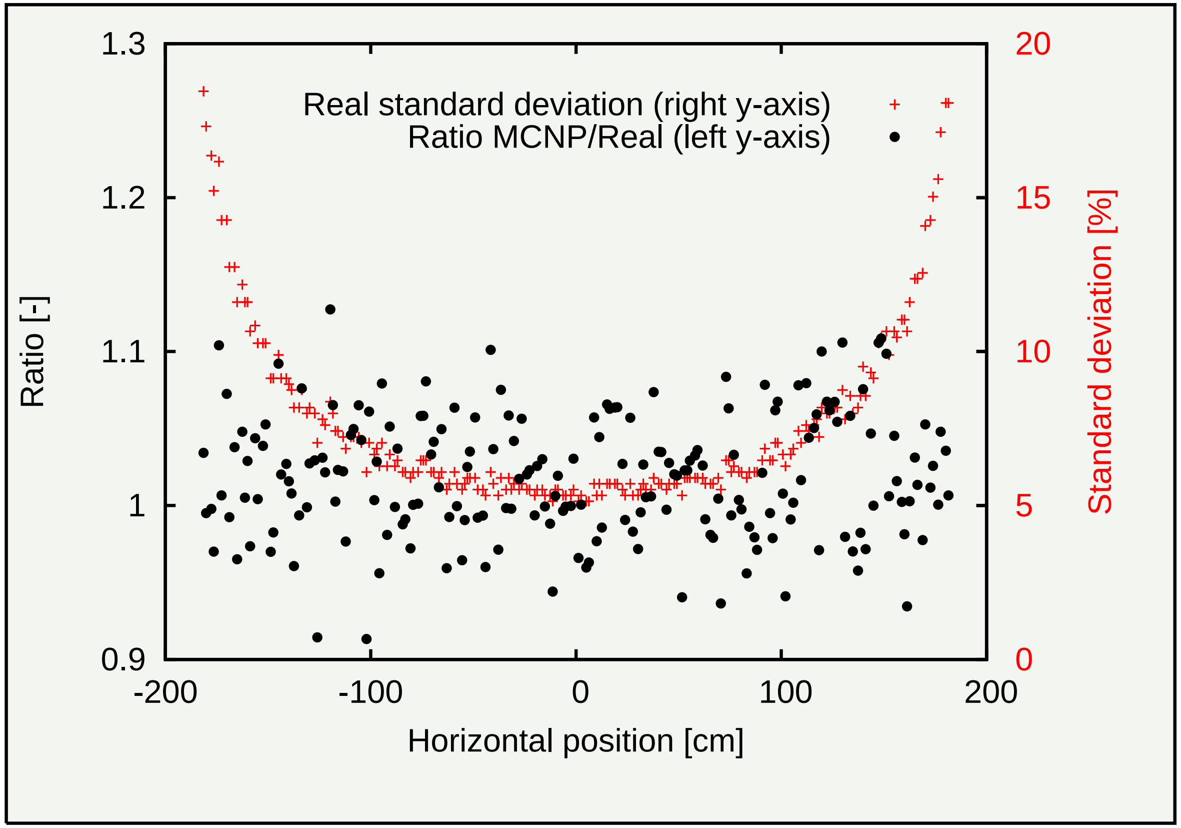
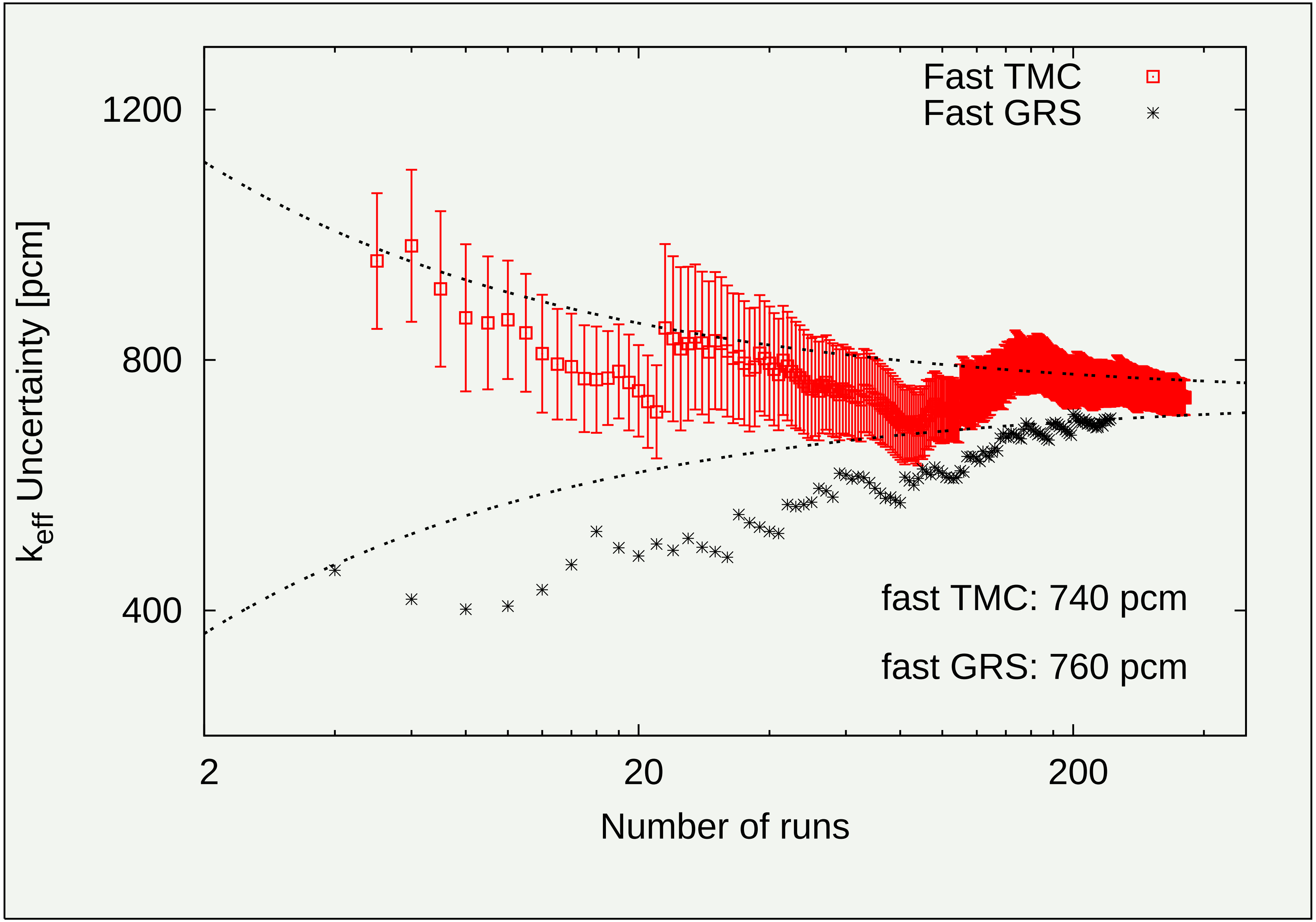
- From the 508 short runs, the first 389 were repeated with fixed nuclear data,
- 274 were then accepted due to source convergence.
- 9 % difference for k_{eff}
- for generated power (f7):

  ratio is 1.019 ± 0.040.

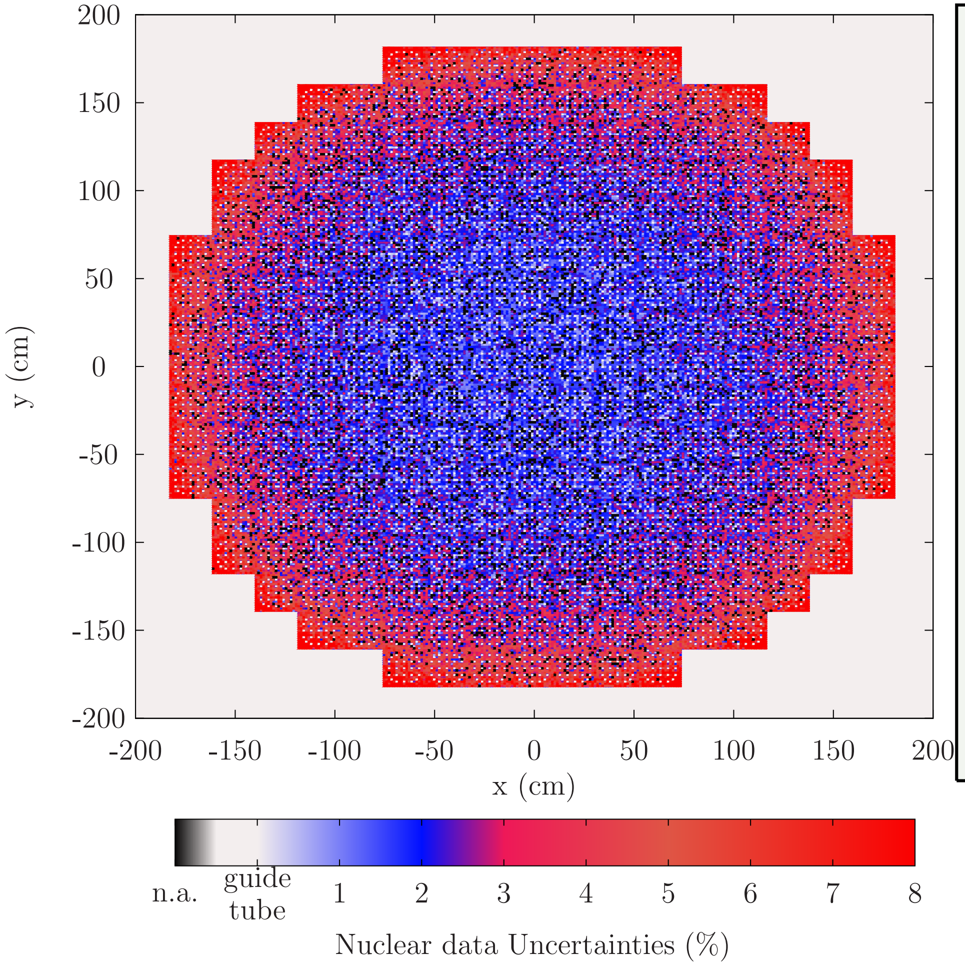


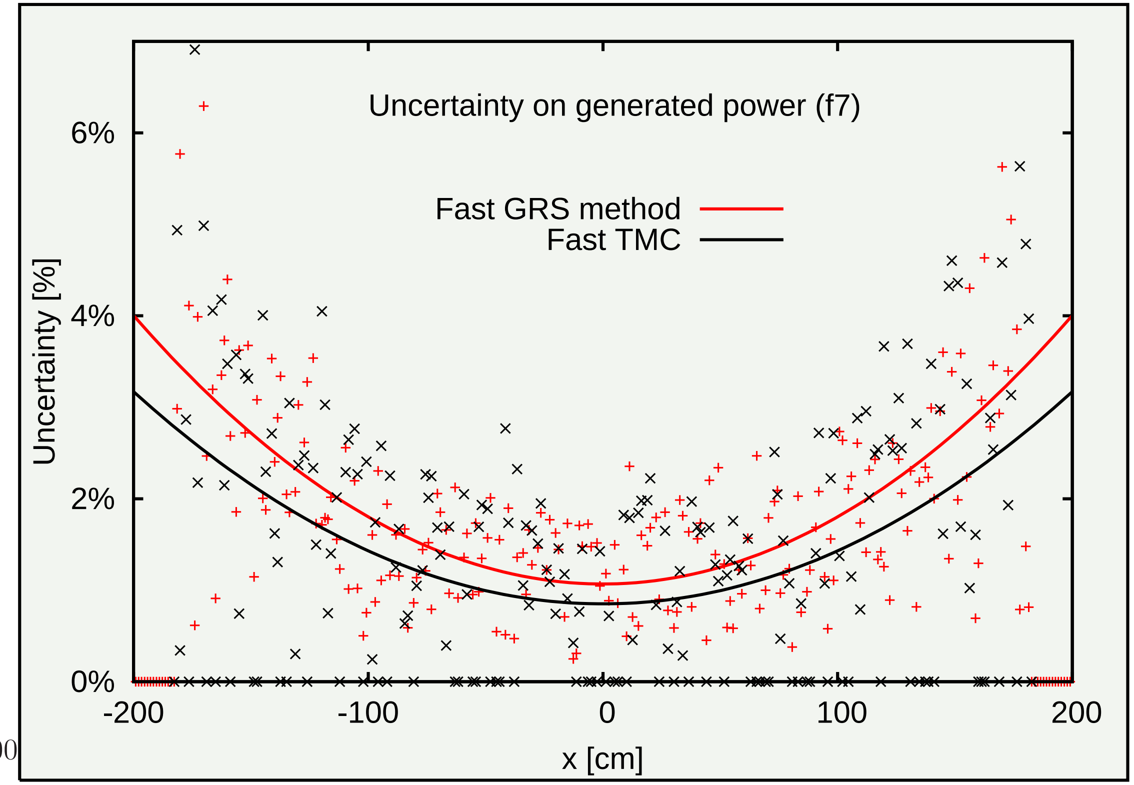
Therefore, for local power, the MCNP estimation of σ_{stat} is good enough.

Fast TMC & GRS methods on a full core: k_{eff} uncertainty



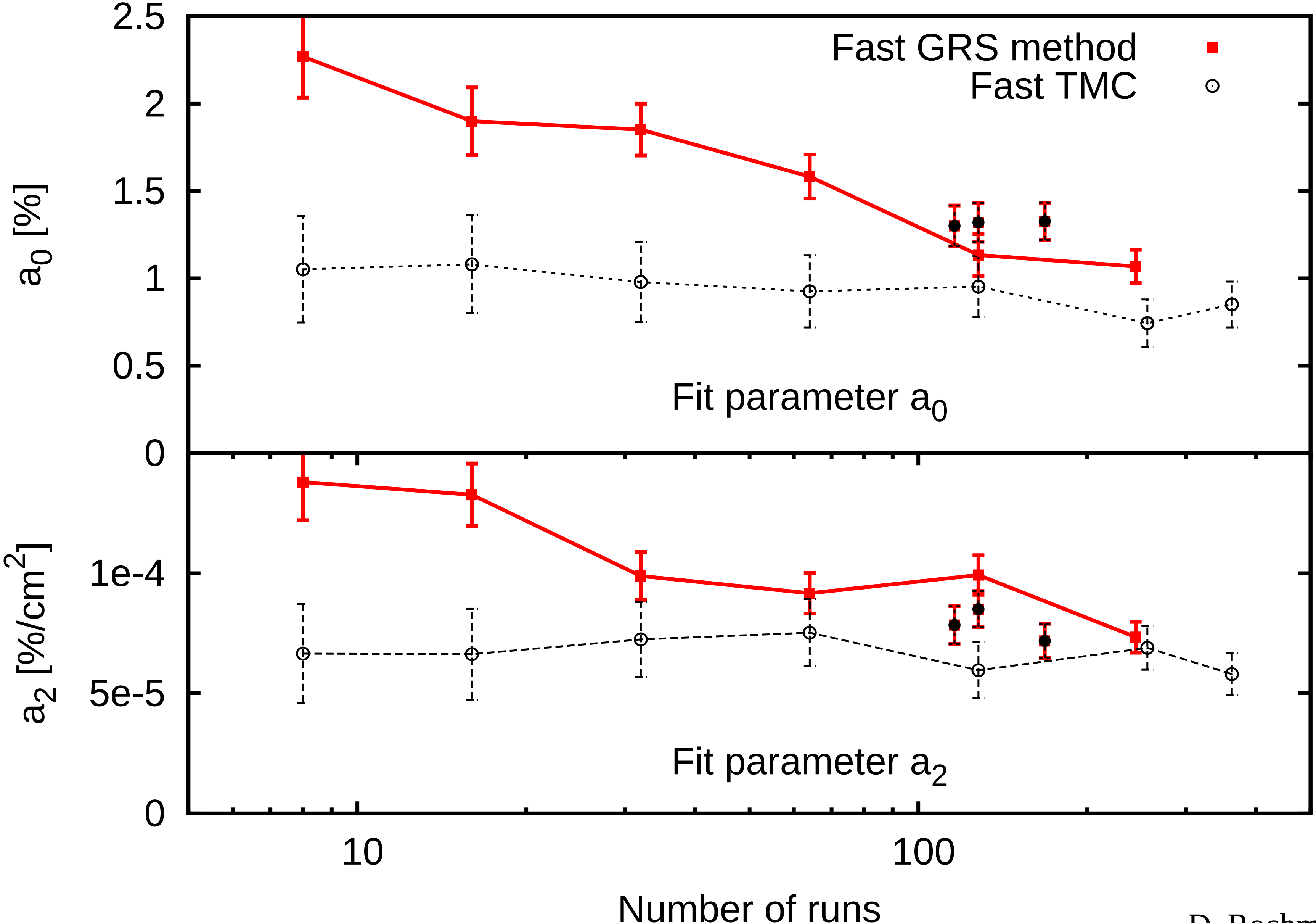
Fast TMC & GRS methods on a full core: generated local power





Fast TMC & GRS methods on a full core: generated local power

- The previous uncertainties can be fitted using $f(x) = a_0 + a_2 x^2$



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fast TMC and GRS methods:
If we can do a calculation once, we can also get nuclear data uncertainties in twice the time (or less).