PAUL SCHERRER INSTITUT

PSI

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Nuclear data uncertainty propagation for reactor and fuel

EPFL, Switzerland, April 6, 2017

Zertifiziertes Managementsystem STARS ISO 9001

Summary

- Introduction

I. Method: Monte Carlo (TMC, BMC)

II. Results with TMC
   1. Criticality-safety benchmarks
   2. PWR Fuel pin keff
   3. Assemblies
   4. Full core
   5. Spent Fuel
   6. Transient

III. Uncertainties from methods

IV. Other uncertainties

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

Are nuclear data important ?

In energy production, better nuclear data can help for:

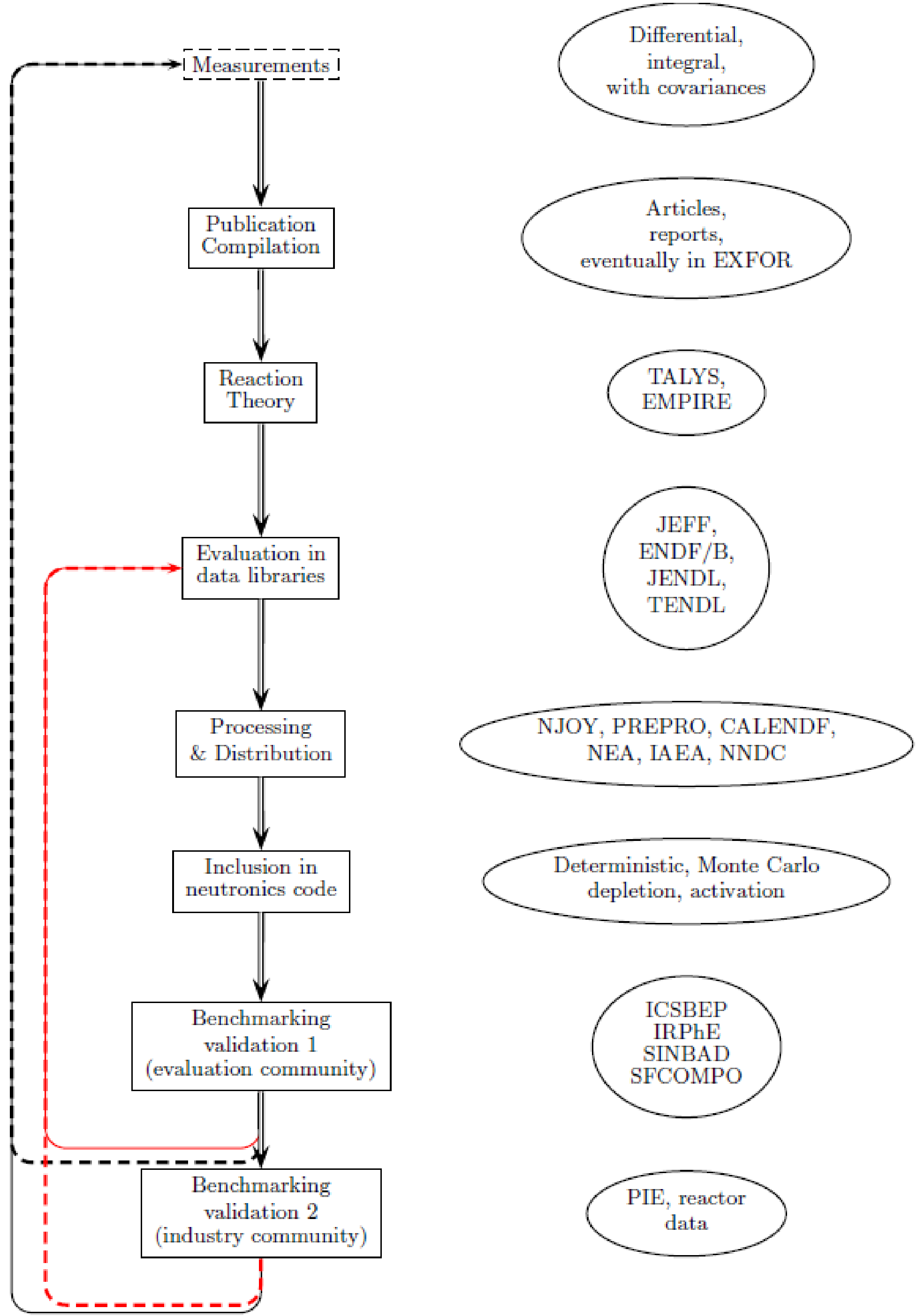
- Fuel storage and processing,
- Life-time extension,
- Outside usual reactor operations,
- Dosimetry,
- Higher fuel burn-up,
- cost reduction in design of new systems,
- Isotope production,
- Shielding (people safety),
- Future systems,

Dry fuel storage, Zwilag, Switzerland

Better nuclear data have a limited effect on:

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

Nuclear data life cycle



Nuclear data uncertainties: general comments

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

Uncertainty ⇌ safety ⇌ professionalism

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

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

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

Uncertainty propagation

Three methods exist today:

1. Based on nuclear data covariance data

- So-called “Sandwich rule” = sensitivity times covariances ,
- Provide uncertainties, sensitivities

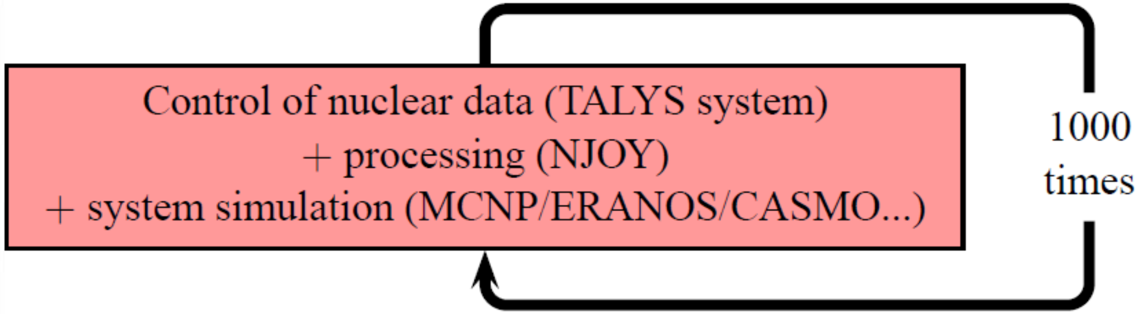
2. Based on nuclear data parameter covariance data:

- So-called TMC (Total Monte Carlo), or BMC (Bayesian Monte Carlo)
- Sampling of model parameters,
- Provide uncertainties,
- Does not provide sensitivities, but importance factors.

3. In between: based on nuclear data covariance data:

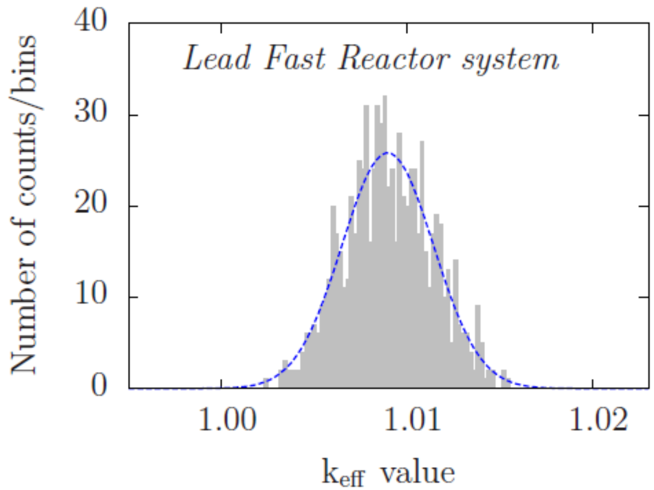
- Sampling of cross section data, based on nuclear data covariances
- Provide uncertainties,
- Does not provide sensitivities, but importance factors,
- Many software: XSUSA, ACAB, NUDUNA, NUSS, SANDY, SAMPLER…

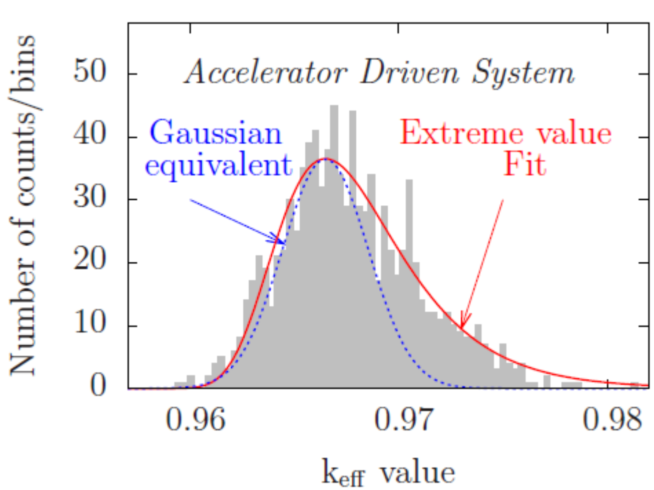
Uncertainty propagation: TMC



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

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





"Towards sustainable nuclear energy: Putting nuclear physics to work",

A.J. Koning and D. Rochman, ANE 35 (2008) 2024.

TMC for nuclear data uncertainty propagation, what else ?

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

☺ + No approximation but true probability distribution,

☺ + Only essential info for an evaluation is stored,

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

☺ + Feedback to model parameters,

☺ + Full reactor core calculation and transient,

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

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

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

☺ + Computer time (not human time)

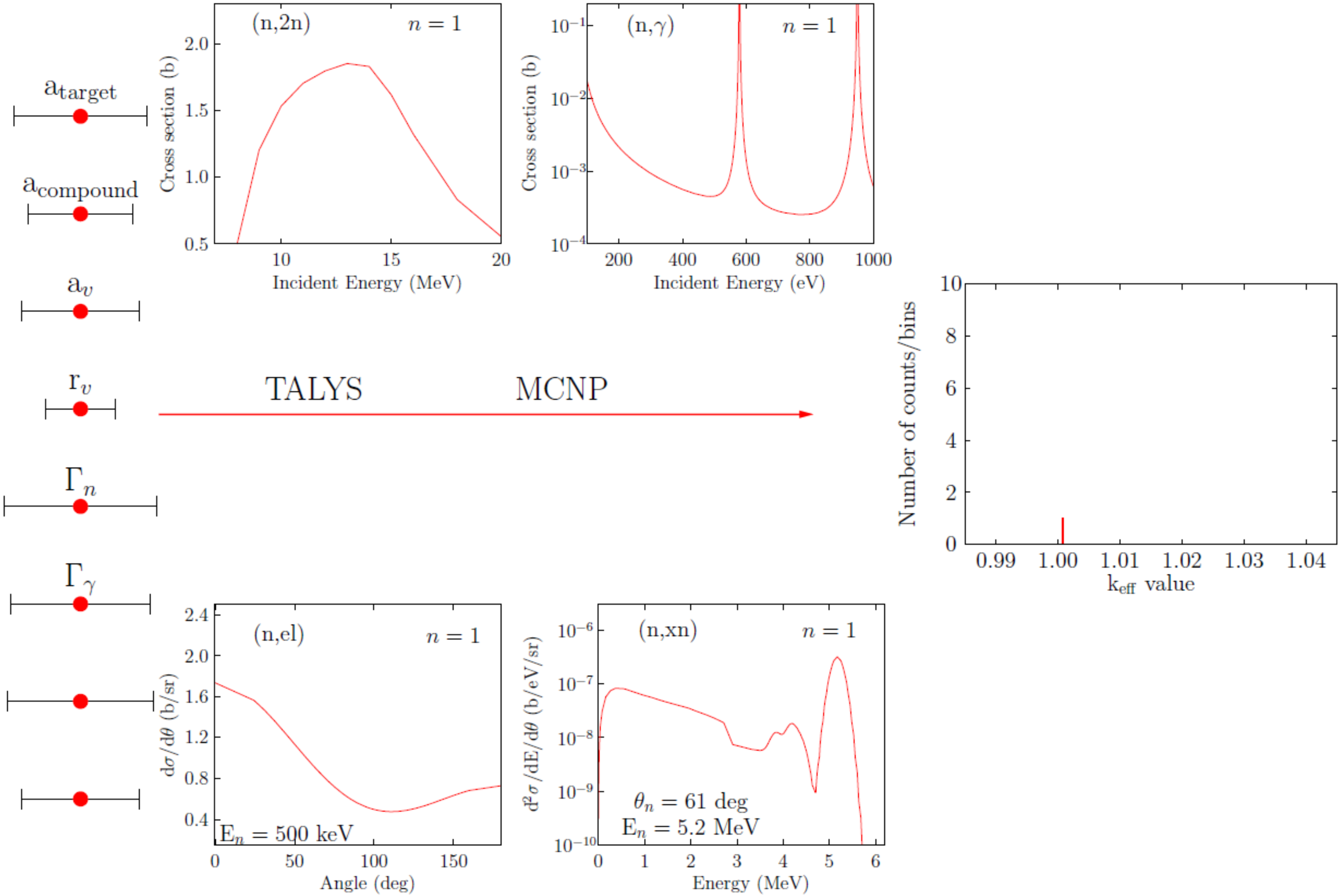
☺ + QA.

☹ - Needs discipline to reproduce,

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

☹ - Need mentality change.

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



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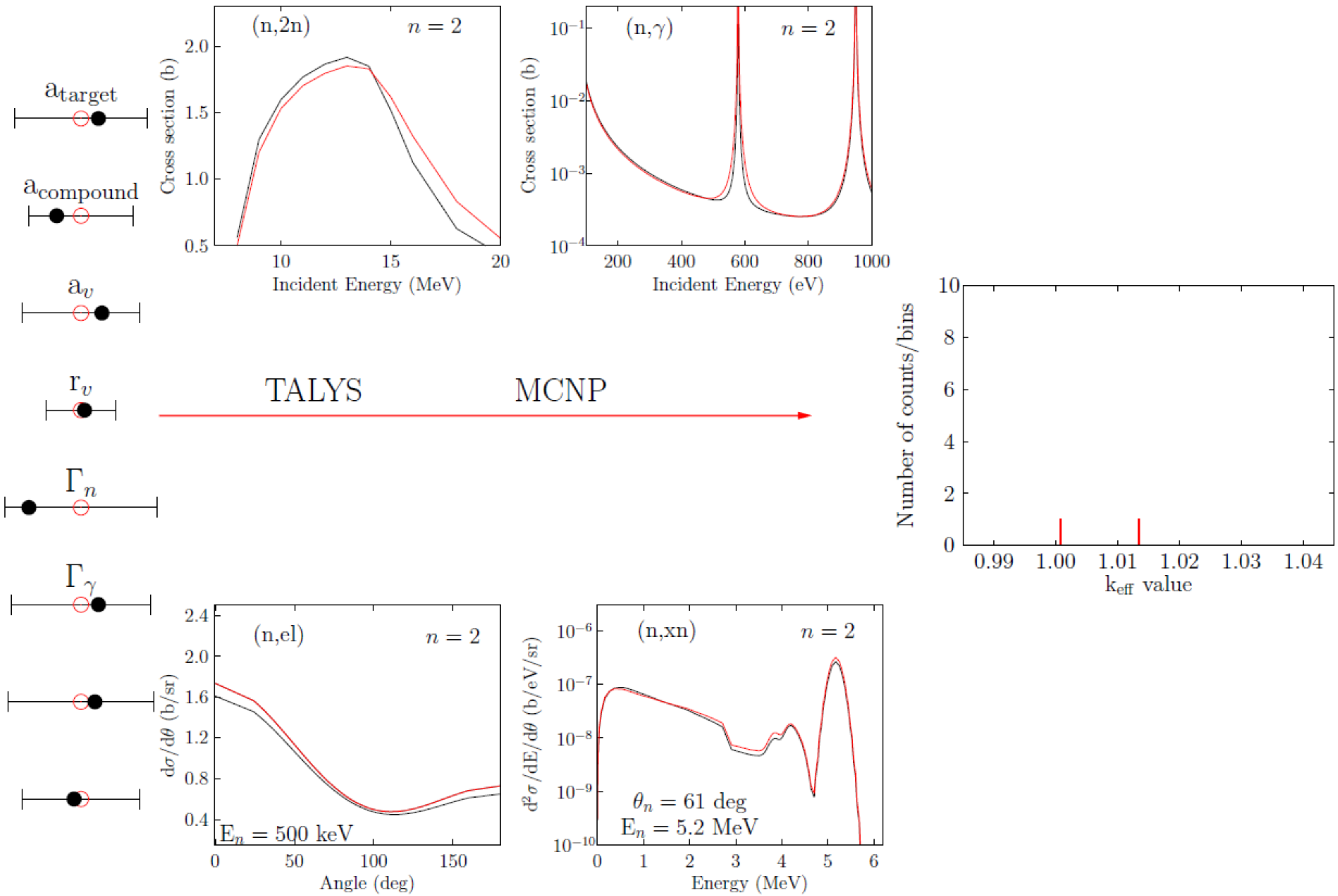

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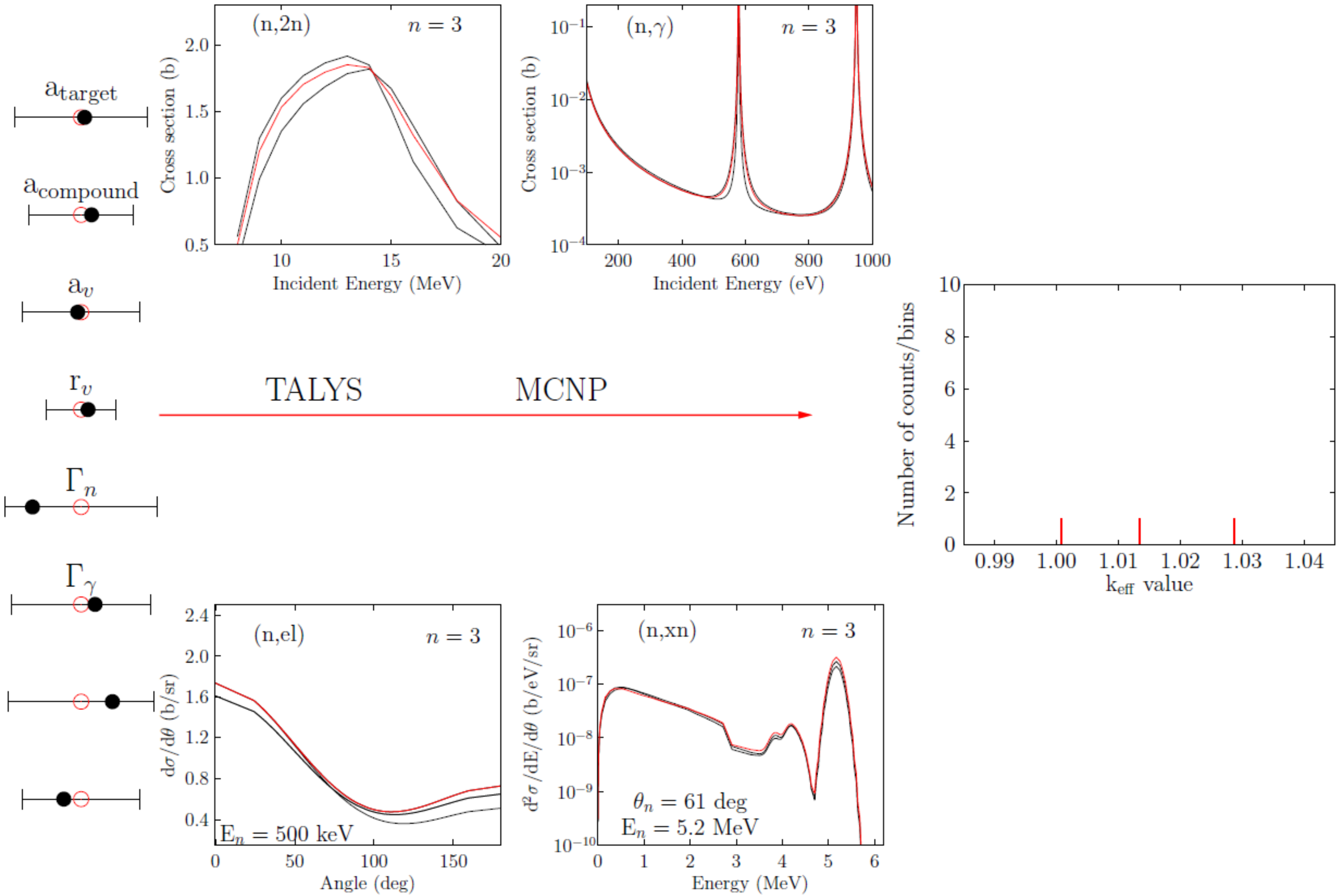

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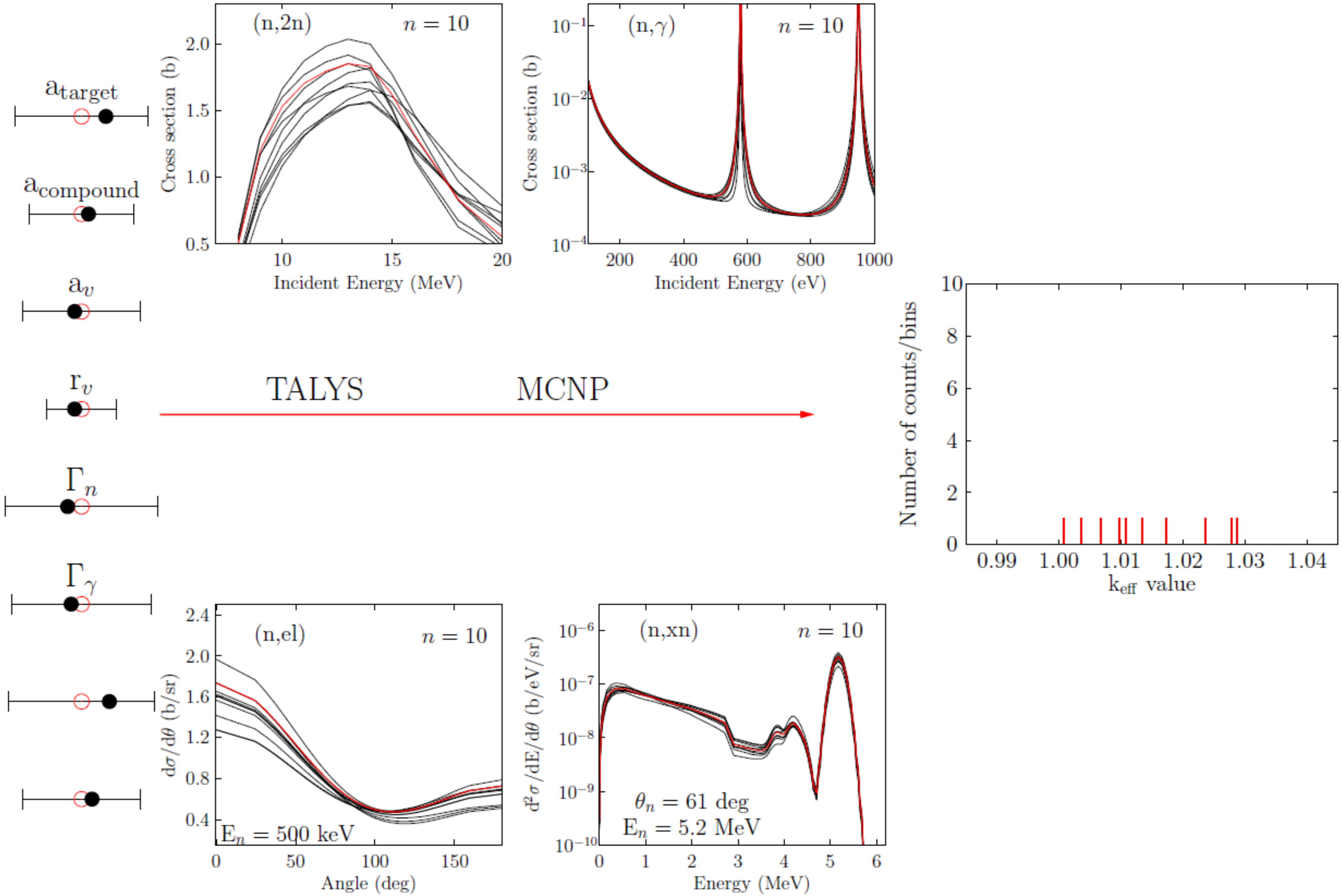

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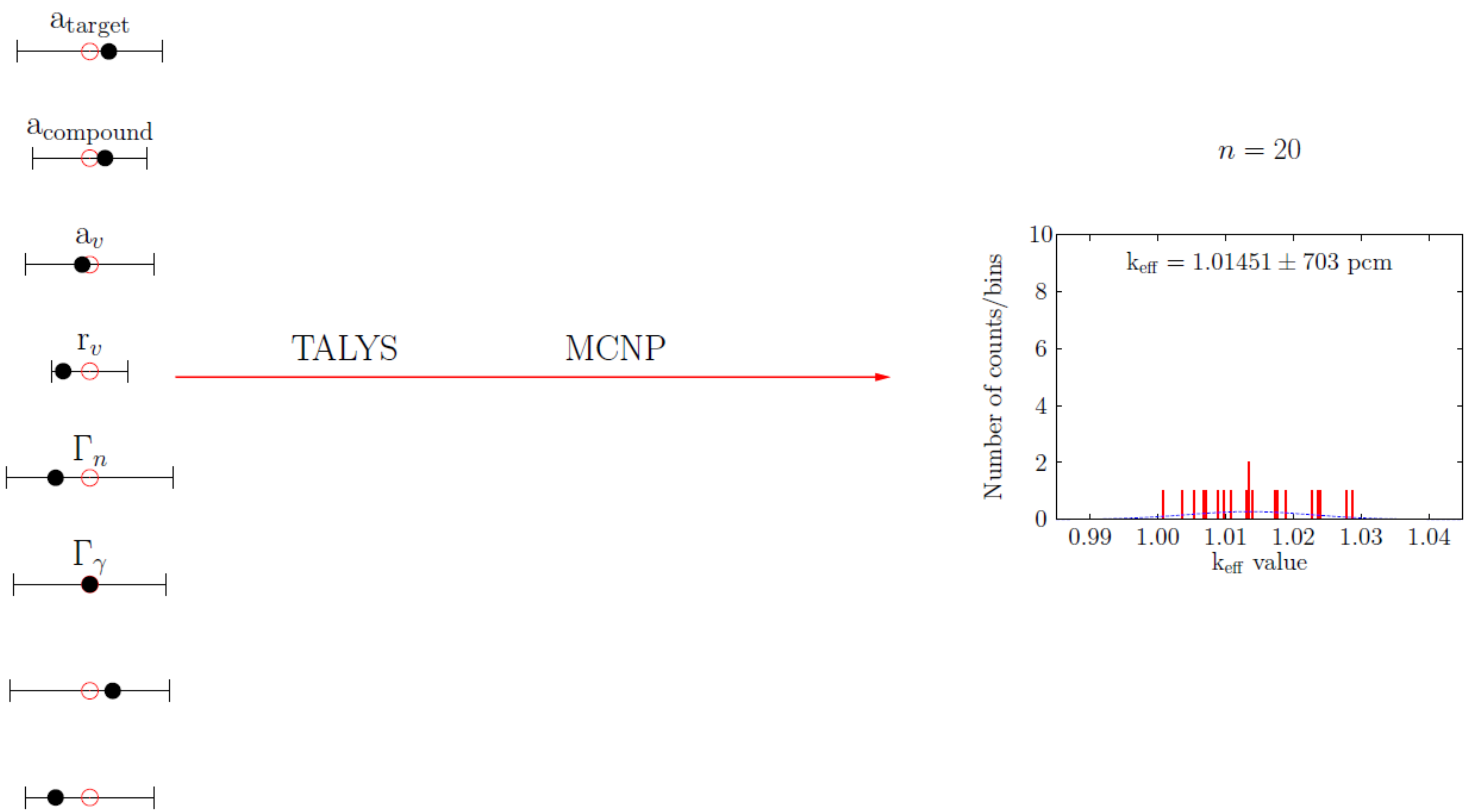

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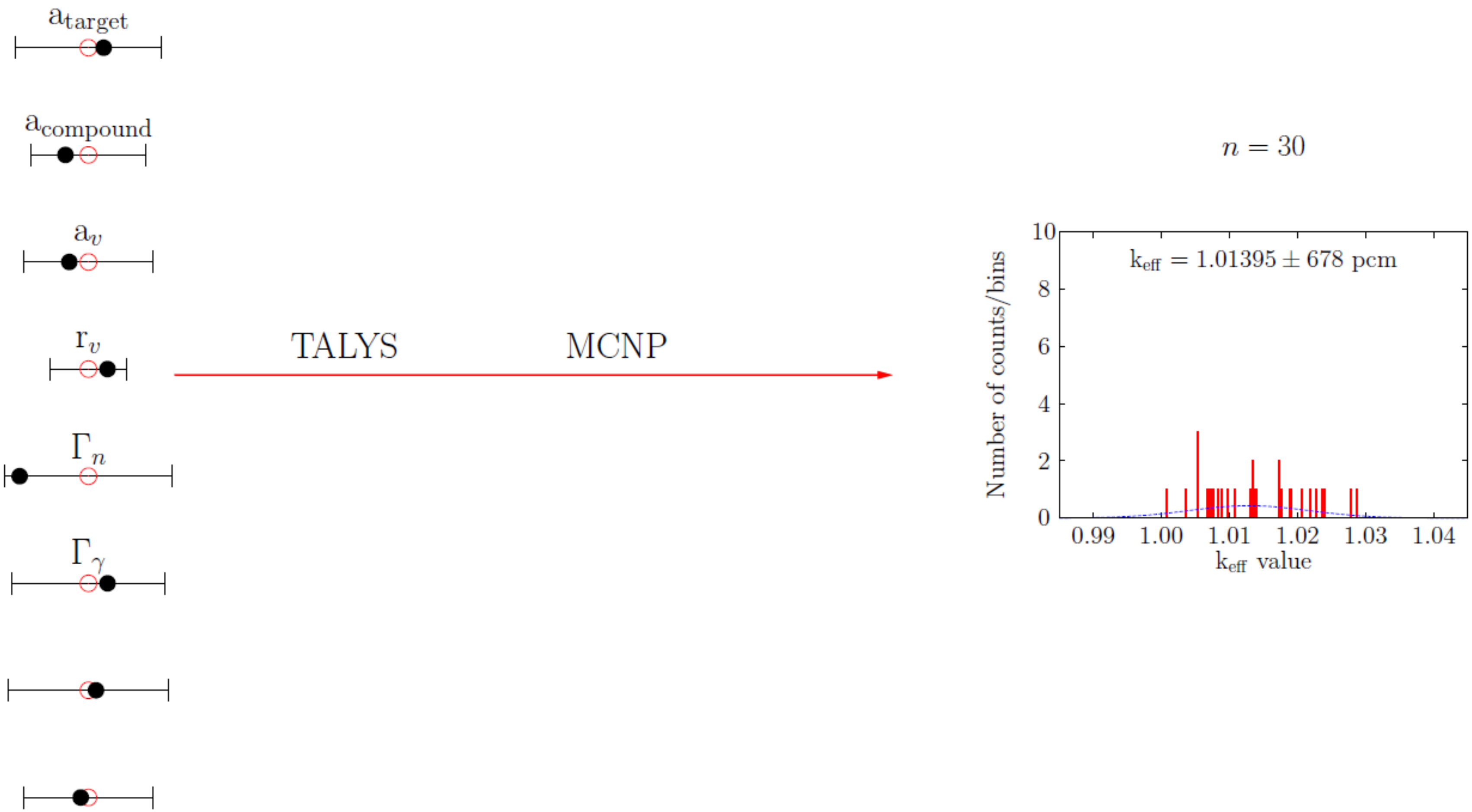

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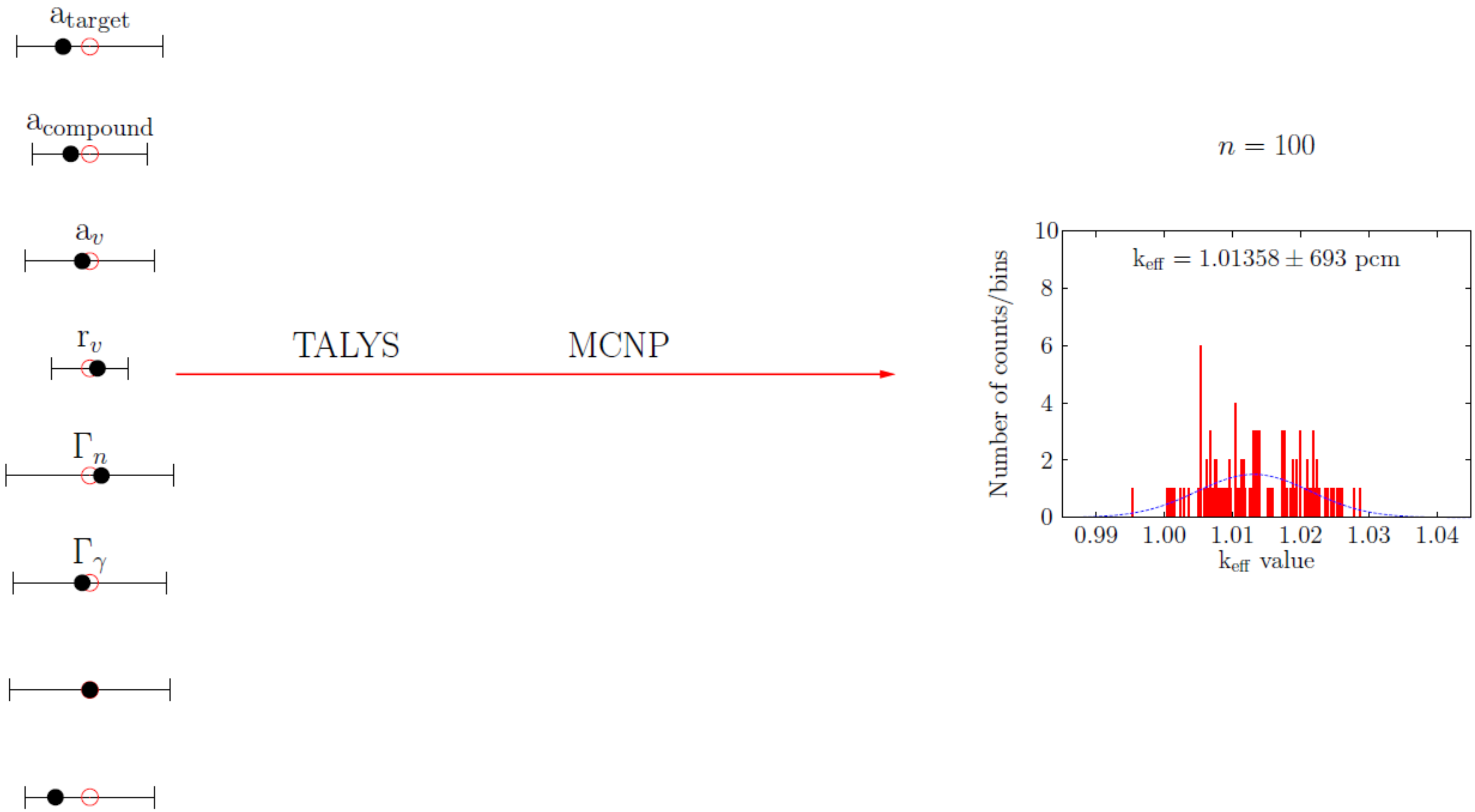

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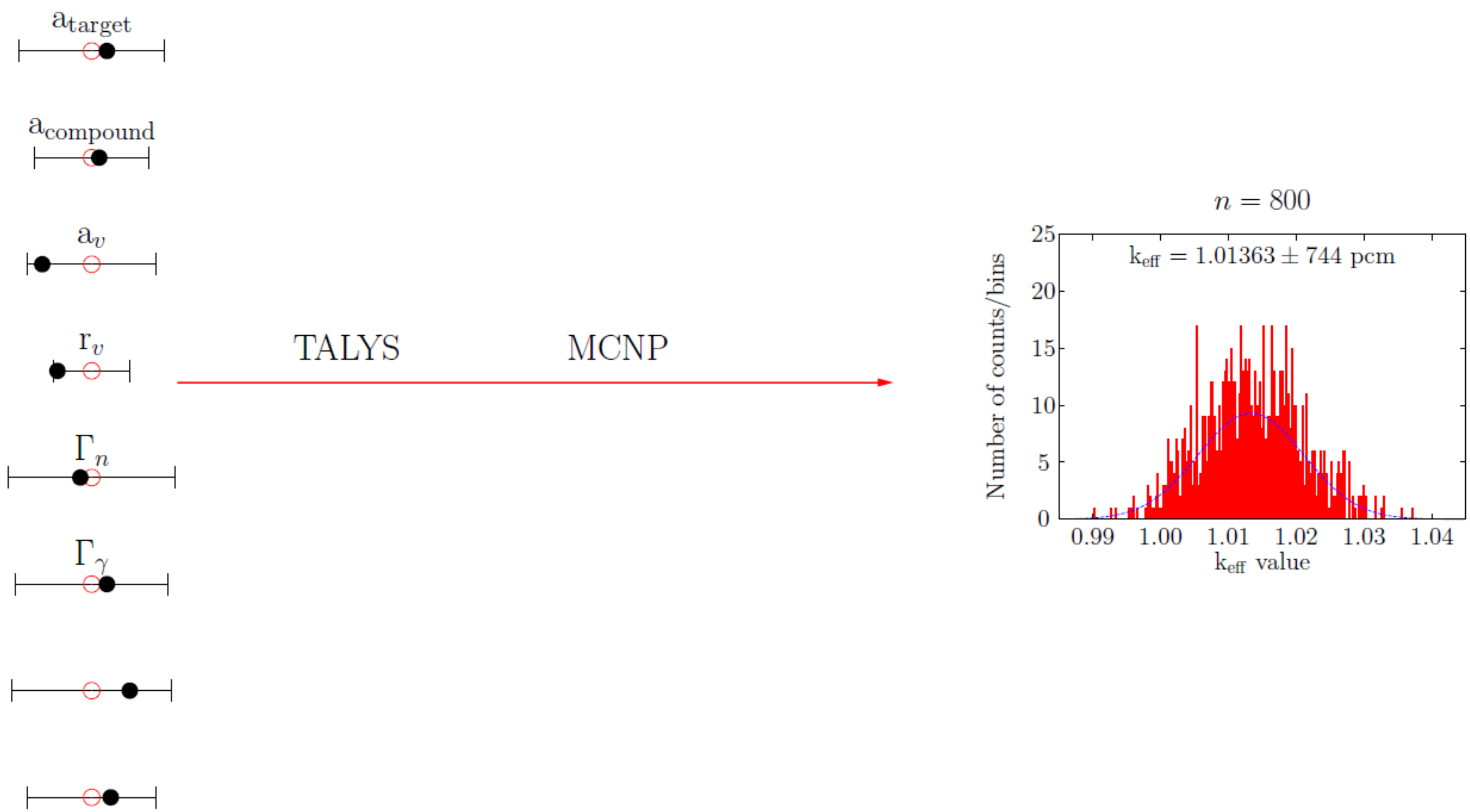

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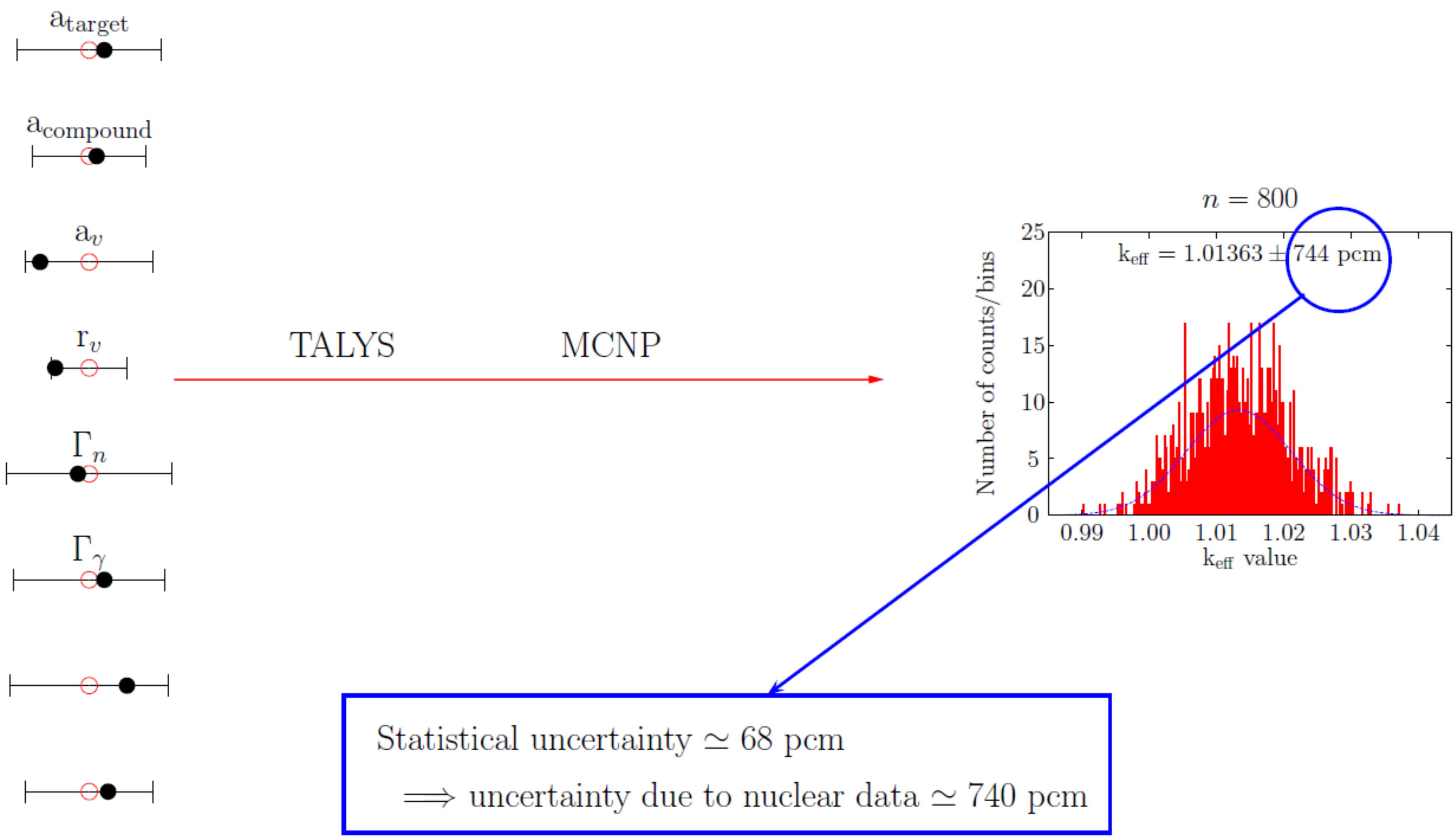
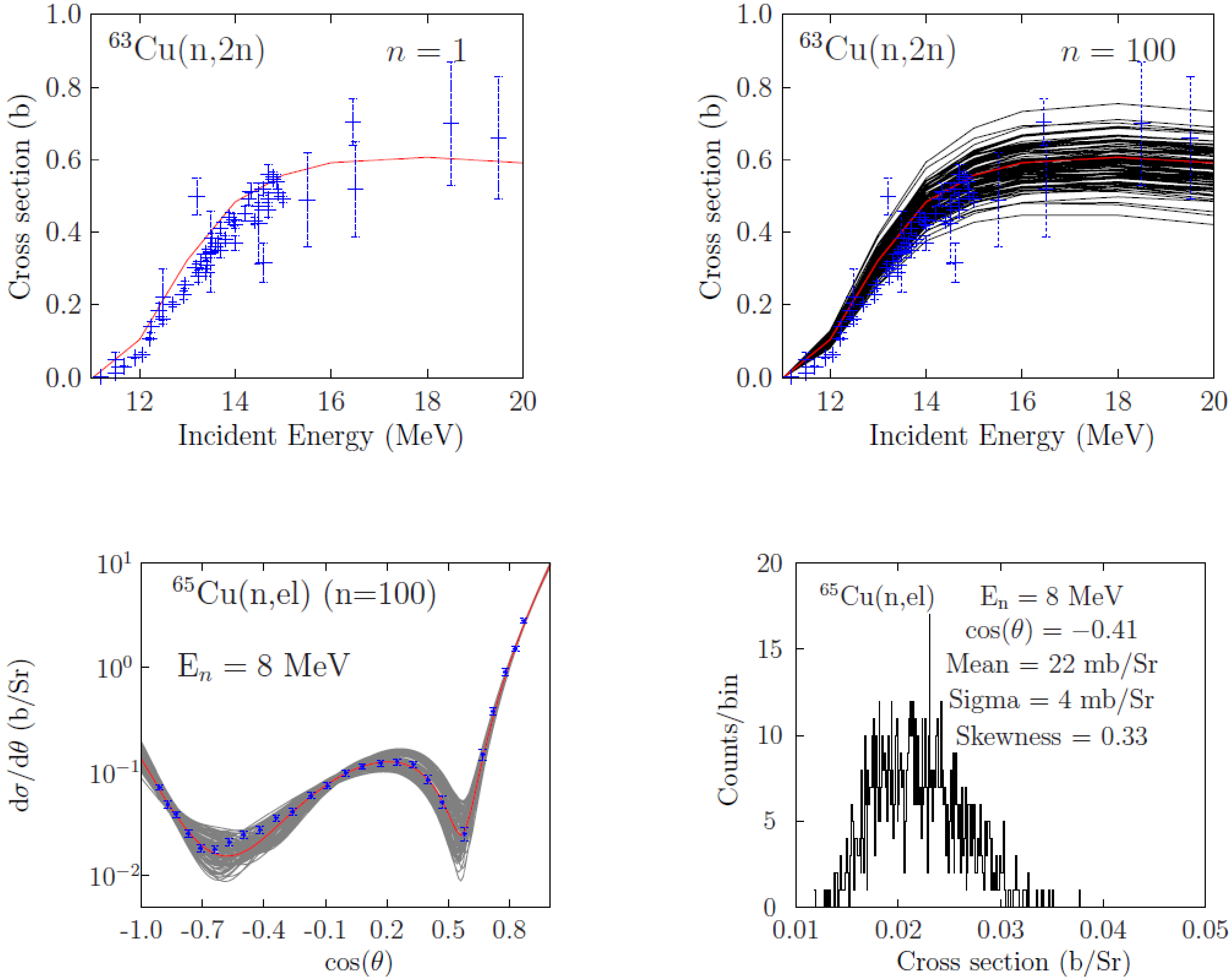
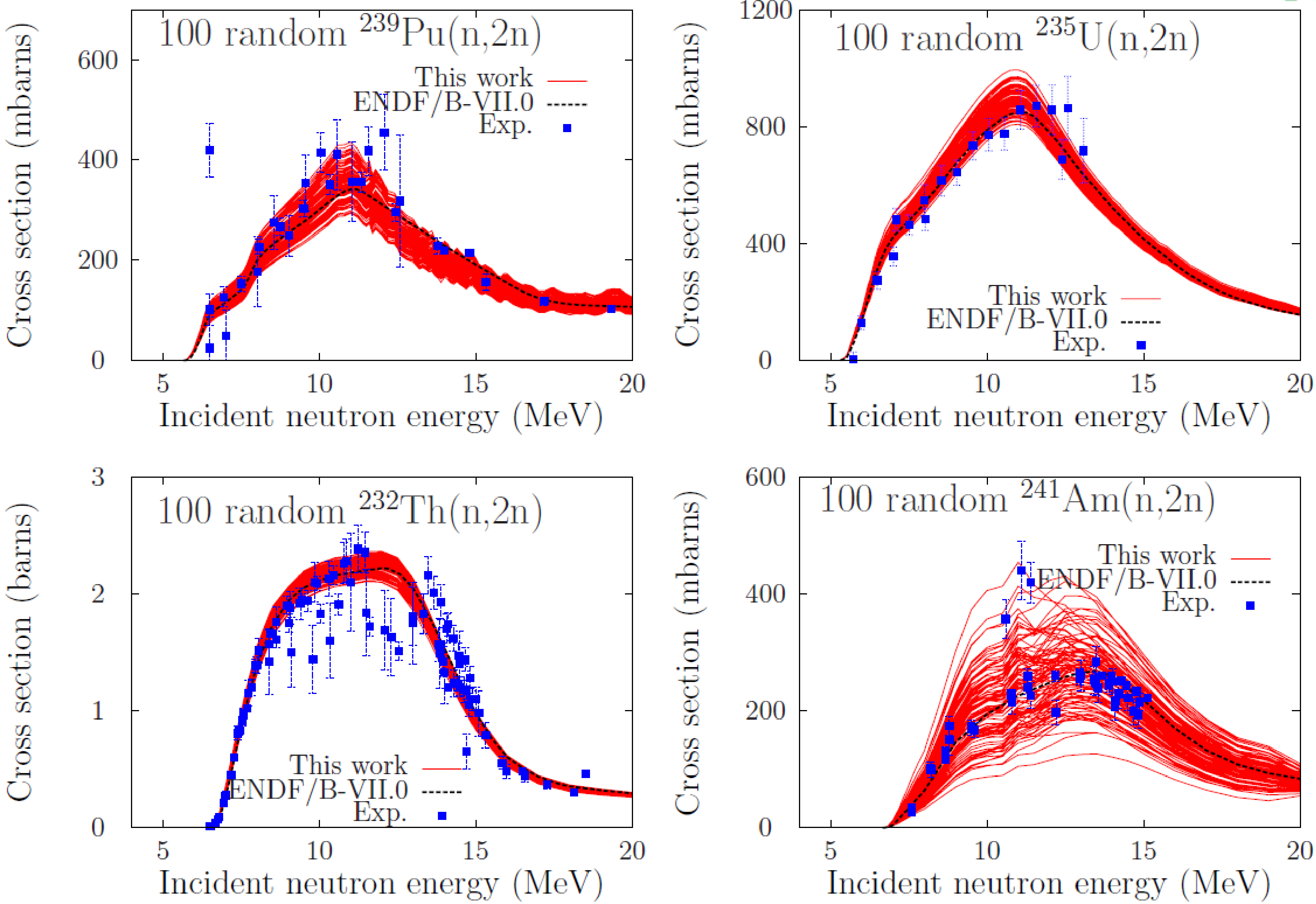


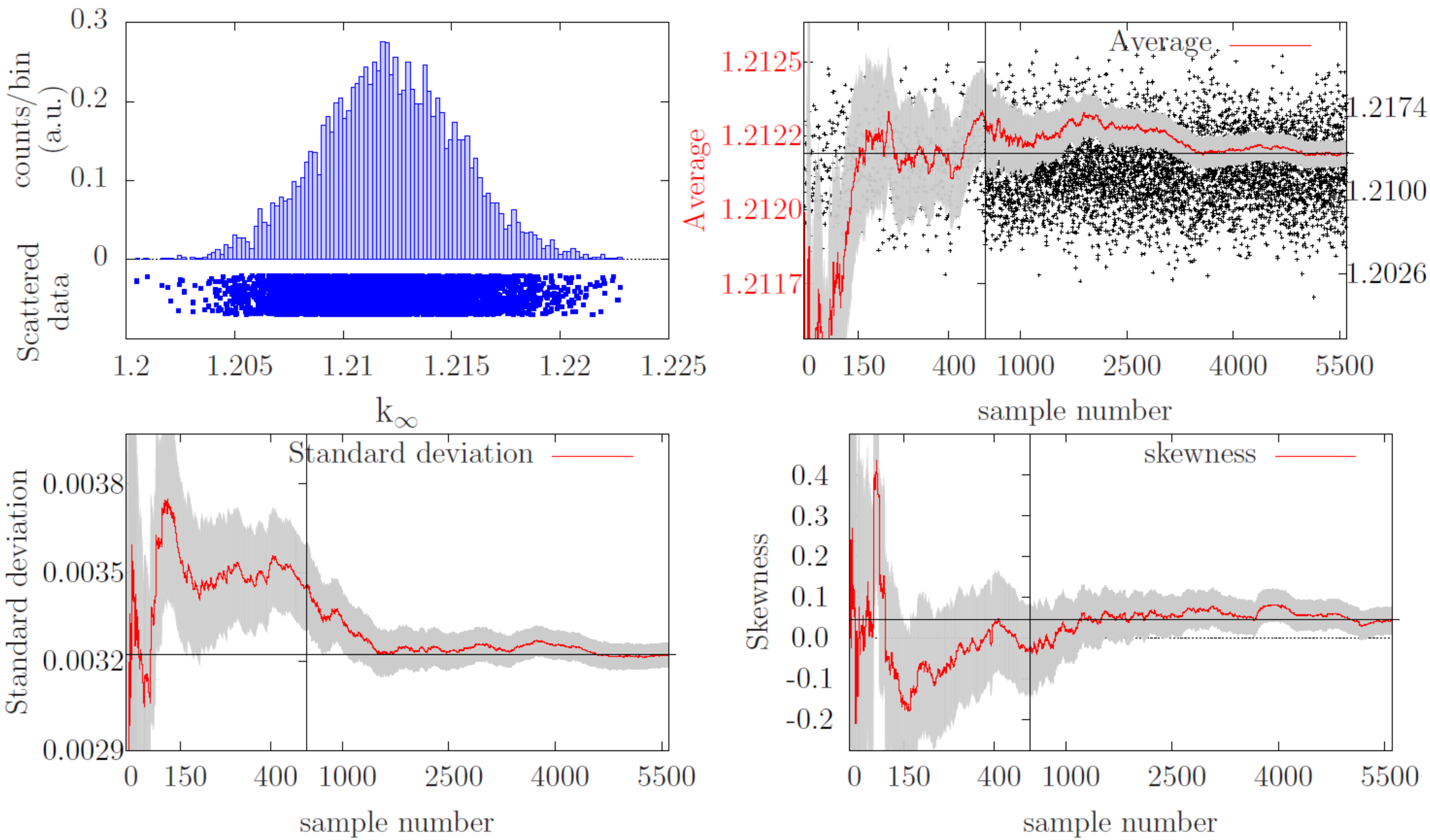
Examples with ^{63}Cu(n,2n) and ^{65}Cu(n,el)



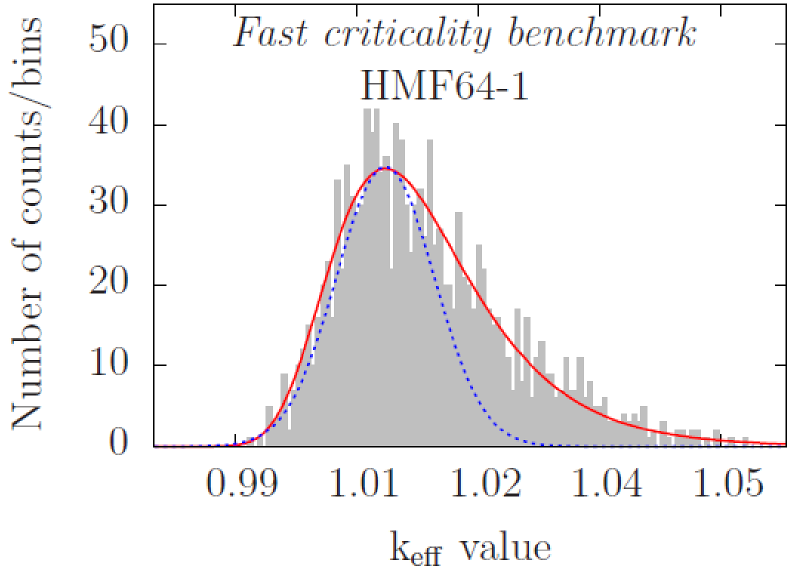
Nuclear data: examples on (n,2n) cross sections

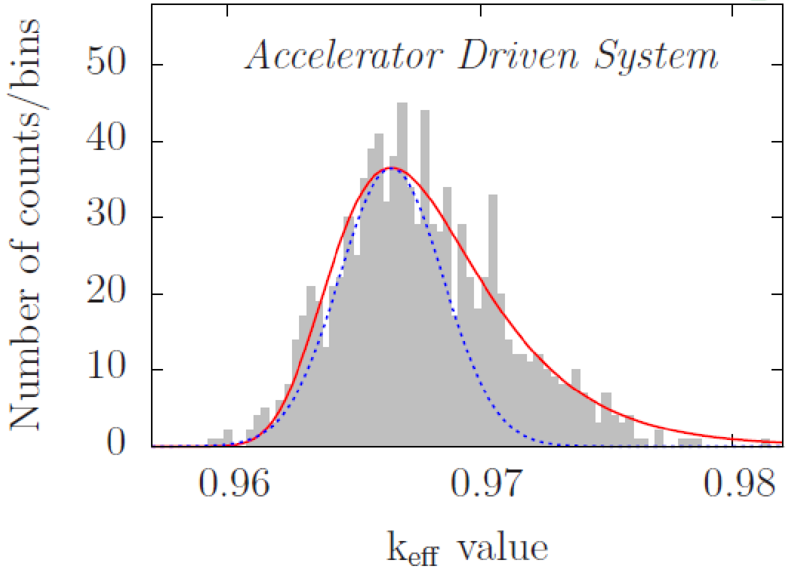


TMC: Convergence of the Monte Carlo process



TMC: No Gaussian assumption





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

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

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

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

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

Remarks TMC

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

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

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

Bayesian Monte Carlo

- The Bayesian Monte Carlo (BMC) is defined as

BMC= TMC + feedback to parameter distributions

- It is also called UMC-B (defined at the IAEA)

- The method works as follows:
  1. Select parameter distributions,
  2. Produce random cross sections by sampling parameters,
  3. Compare to EXFOR: calculate a χ^2
  4. use weights to update the parameter distributions
  5. Sample again and calculate new χ^2
  6. (Repeat 3 to 5 until convergence)

BMC

- TALYS parameters are used
- Normal and independent distributions, X^2 defined as

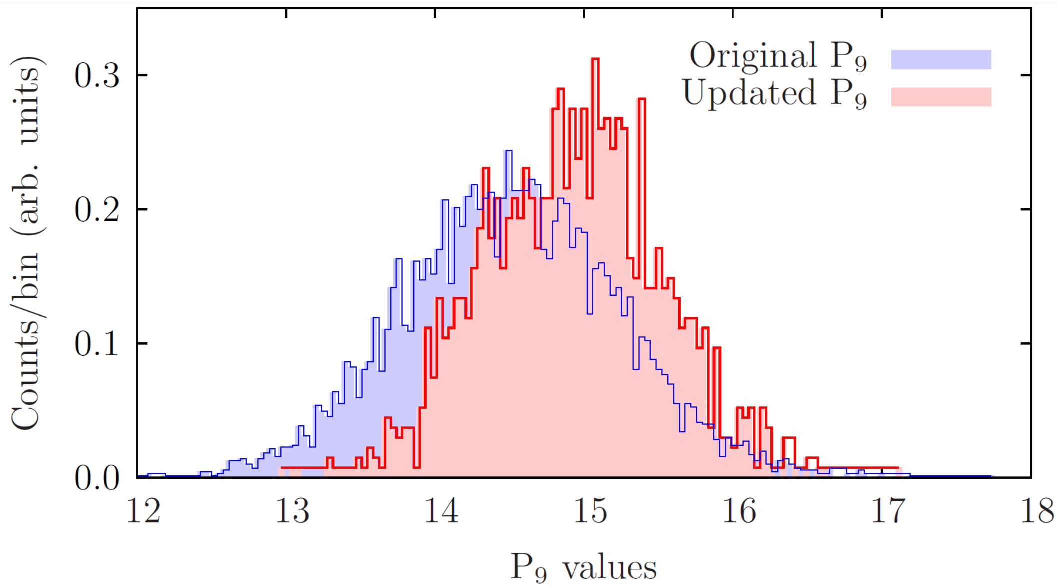
$$\chi_i^2 = \sum_{j=1}^{FY} \left(\frac{C_j^{(i)} - E_j}{\Delta E_j} \right)^2$$

i random calculation

- Weights defined as

$$\omega_i = \frac{e^{-\chi_i^2/2}}{e^{-\chi_{min}^2/2}}$$

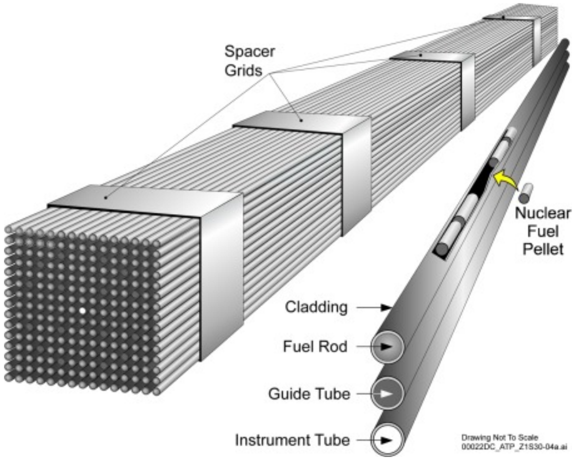
- Example for a specific parameter (P_9=P_AWidth for $^{235}U + n_{th}$)

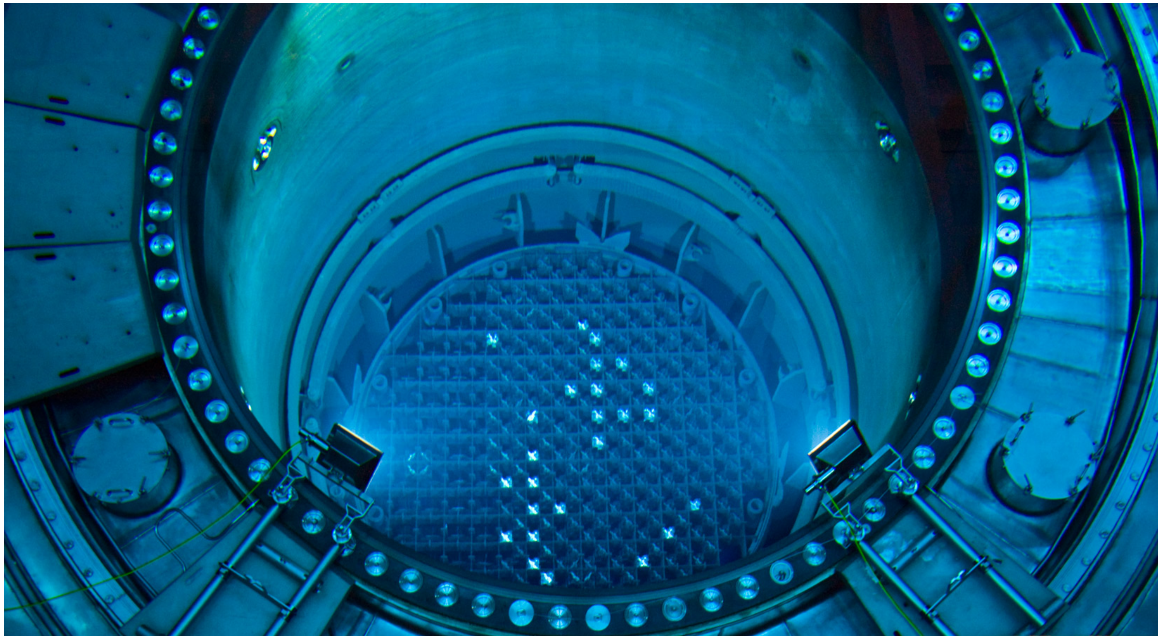


Results 2. PWR Fuel pin

All starts with a pincell:

- Assembly simulations start with pincell simulations,
- Core simulations start with assembly simulations,
- Fuel storage simulations start assembly simulations,





Results 2. PWR Fuel pin

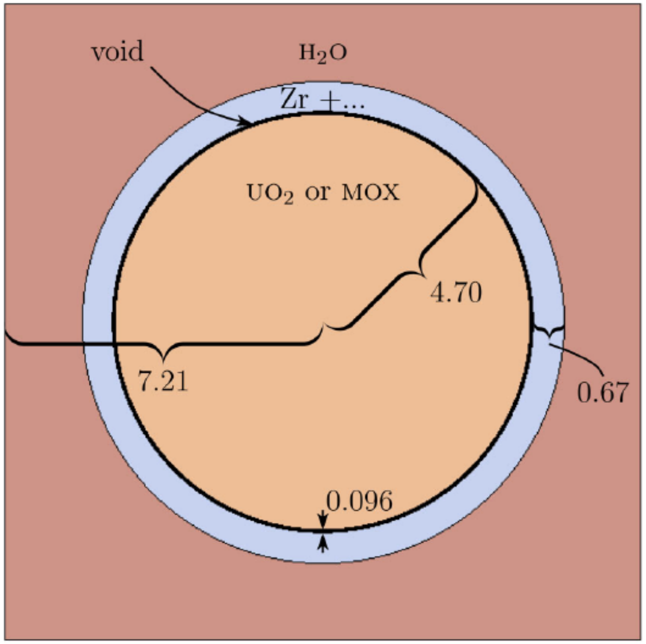


Fig. 1. The geometry of the pin cell model used in Serpent. The fuel, either UO_2 or MOX, is surrounded by concentric annular rings with a void and Zircaloy clad. The rest of the square is filled with water, and all sides are subject to reflecting boundary conditions. All distances are in millimeters.

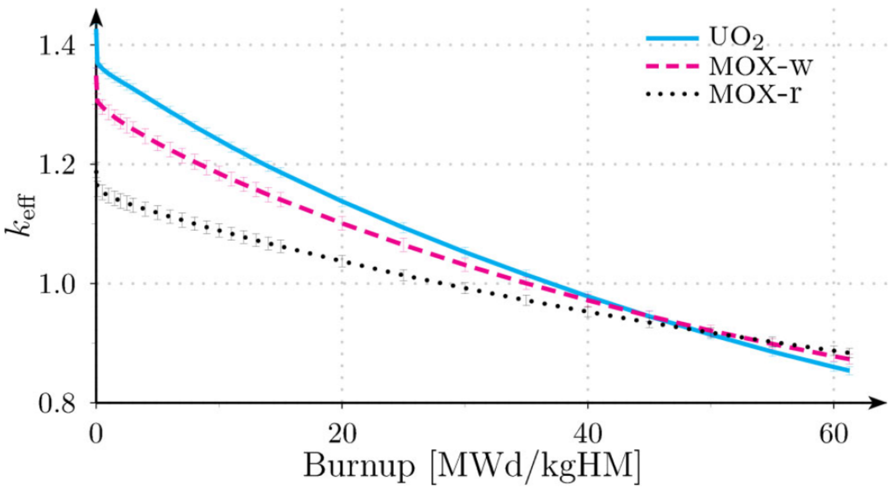


Fig. 3. $k_{\text{eff}} = k_\infty$ as a function of burnup for the three fuel types. The large deviations from 1 are explained by the simplified model: no leakage, infinite grid of pin cells (with the same burnup), and no control mechanisms. The uncertainty bars represent the data uncertainty $\sigma_{data}(k_{eff})$; the statistical uncertainty is negligible in comparison.

Results 2. PWR Fuel pin

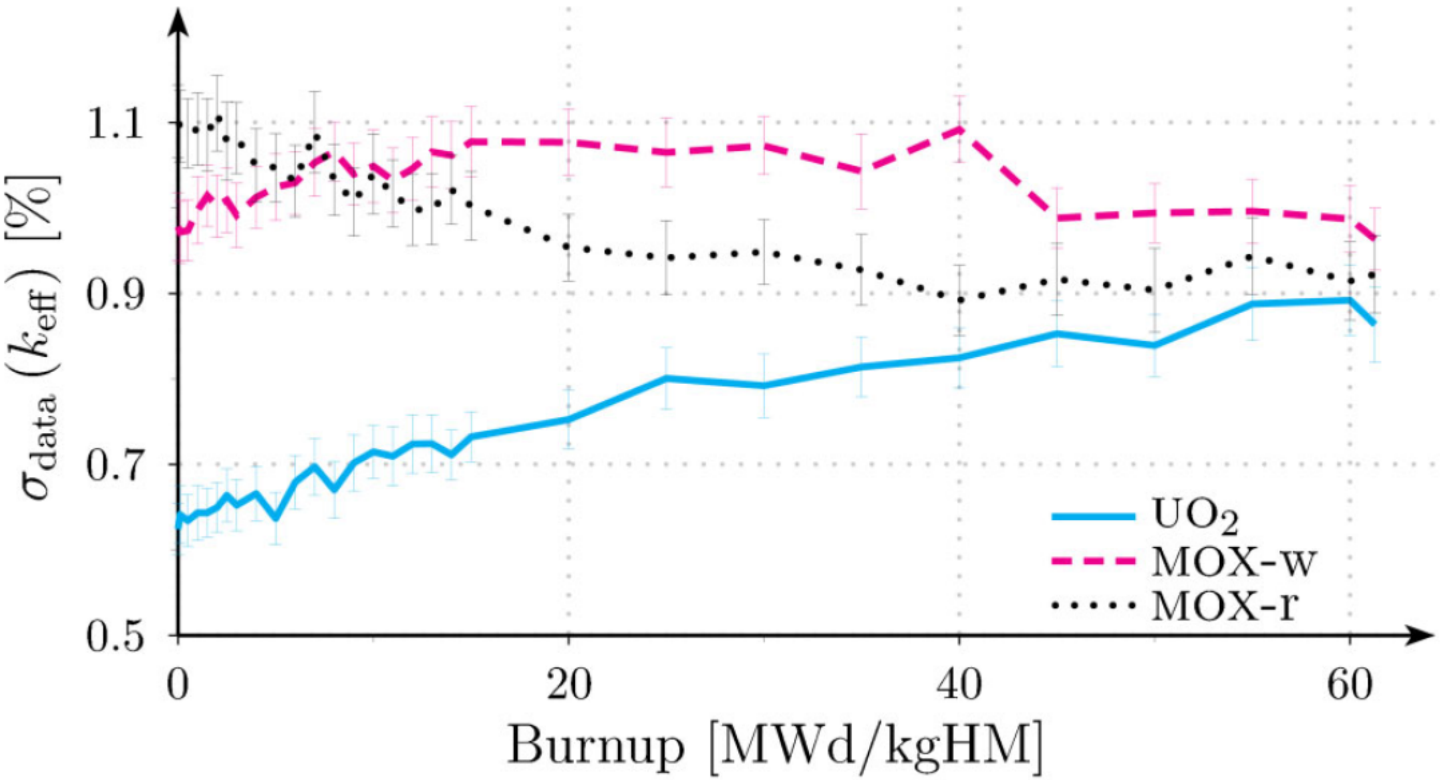


Fig. 2. The main result: Propagated data uncertainty in k_{eff} for UO_2 and the two types of MOX fuel as functions of burnup due to all data. The uncertainty bars represent one standard deviation.

Results 2. PWR Fuel pin

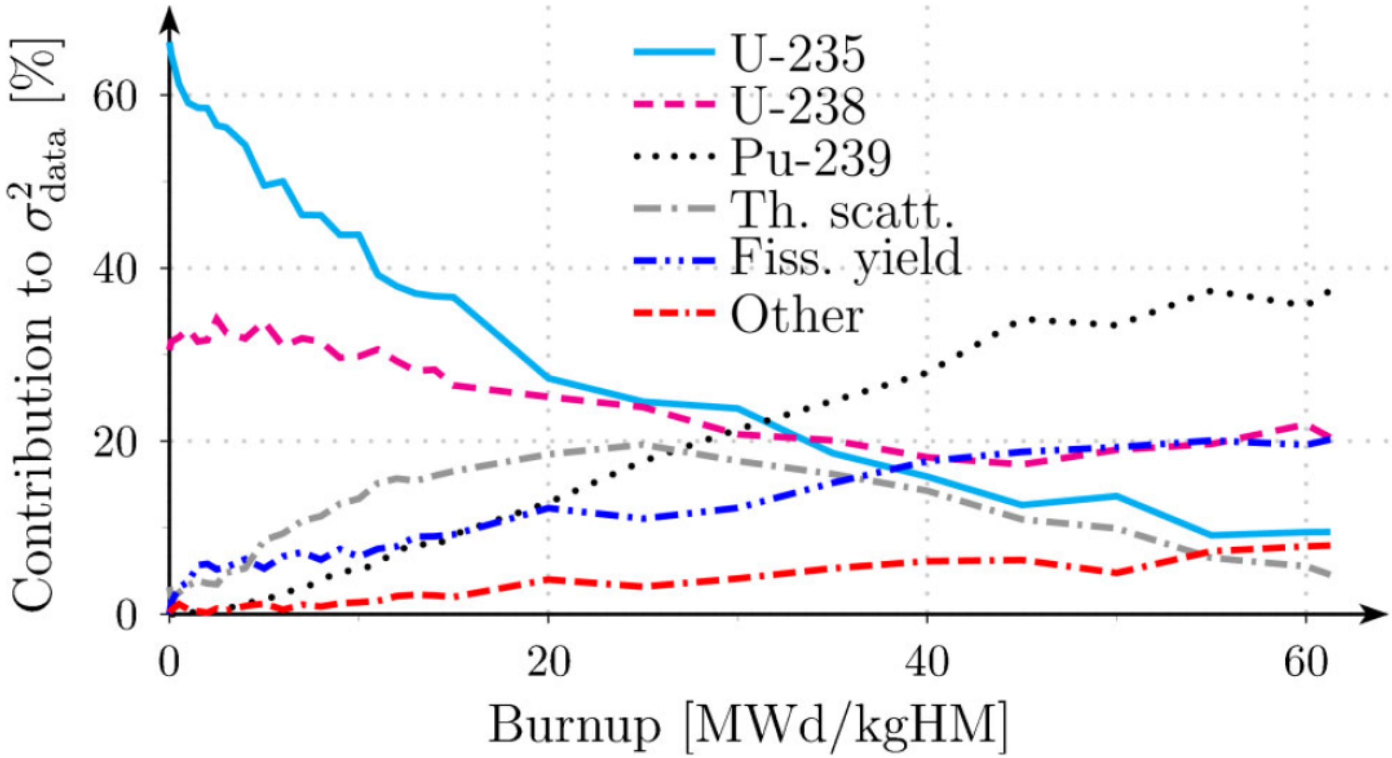
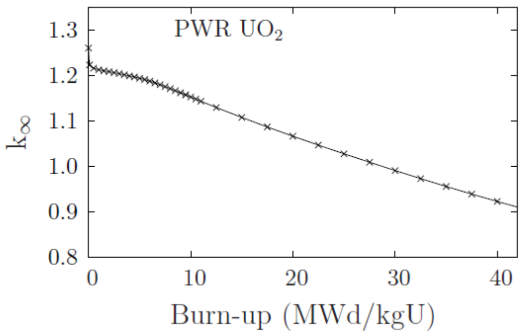
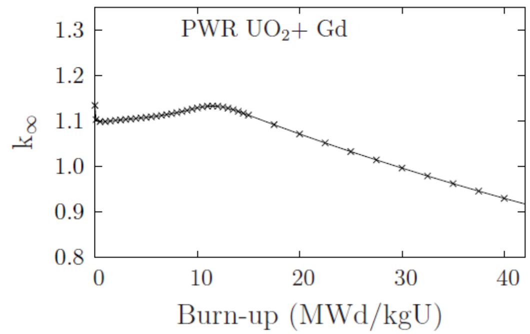


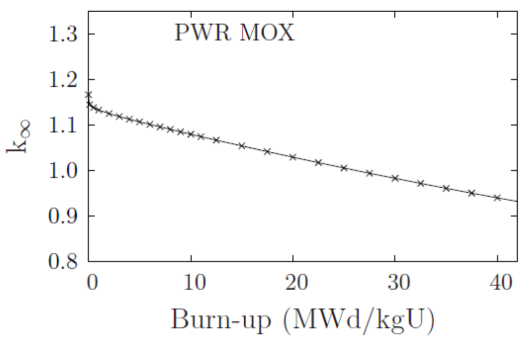
Fig. 4. Contributions to total variance in k_{eff} from variance of individually varied data, for UO_2. "Other" stands for transport and activation data of fission products and minor actinides.

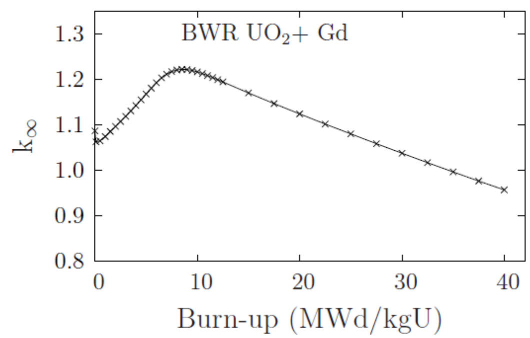
Results 3. Assembly

- Different types of assemblies exist: e.g. PWR, BWR, with UO_2, MOX
- It leads to different uncertainties
- Only 2D models are usually used

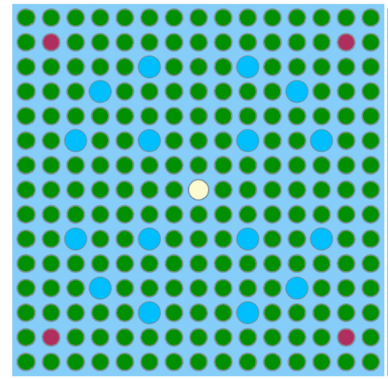




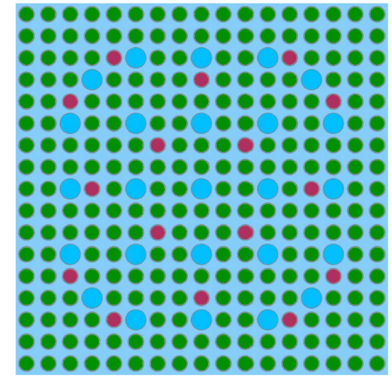




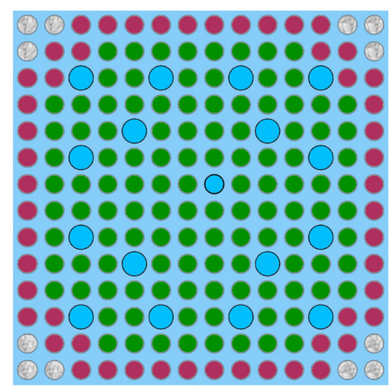
PWR UO_2



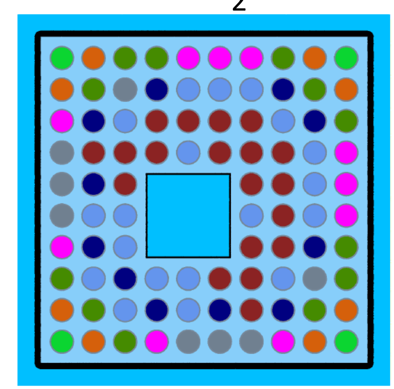
PWR UO_2 + Gd



PWR MOX

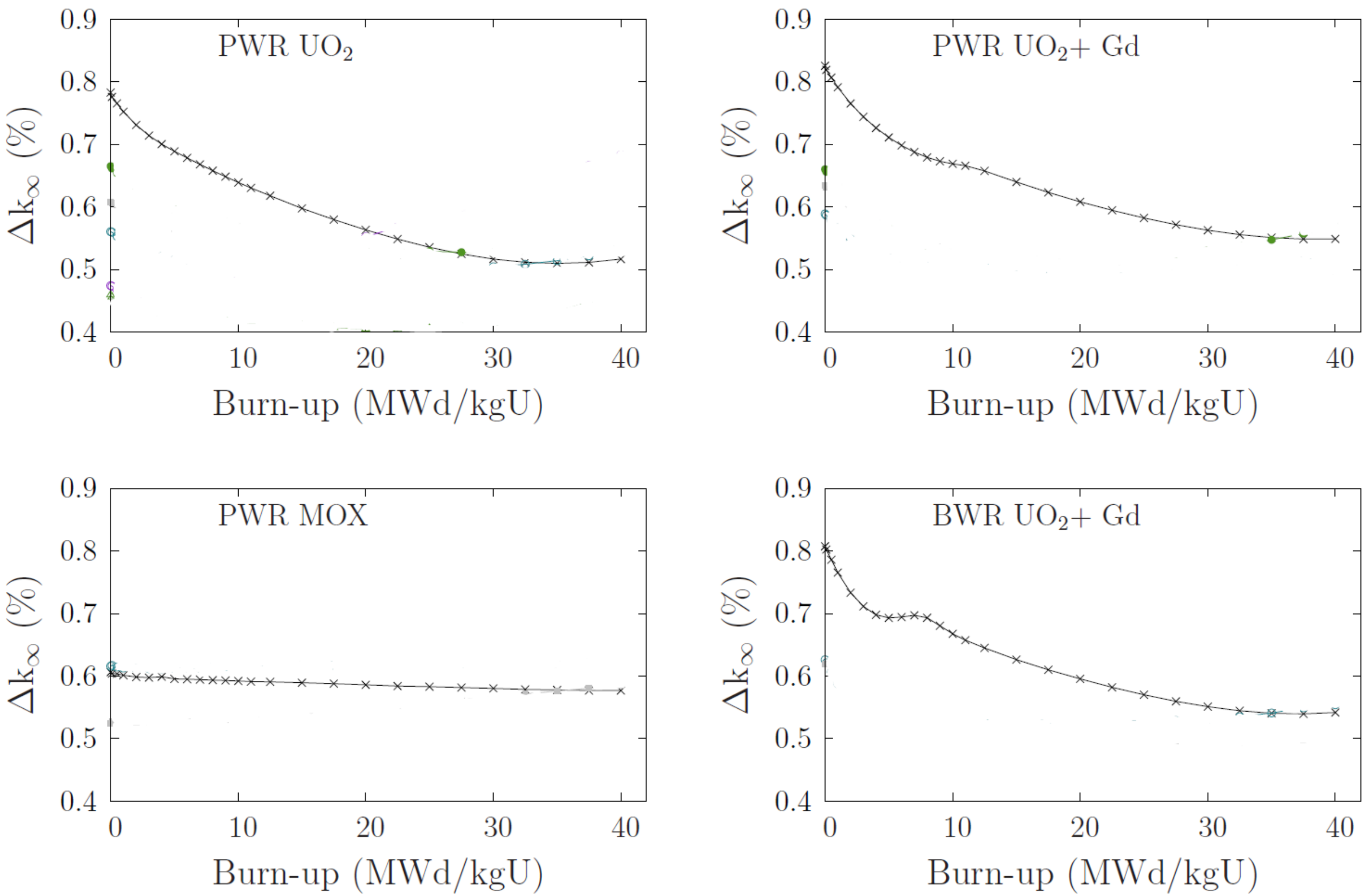


BWR UO_2+ Gd



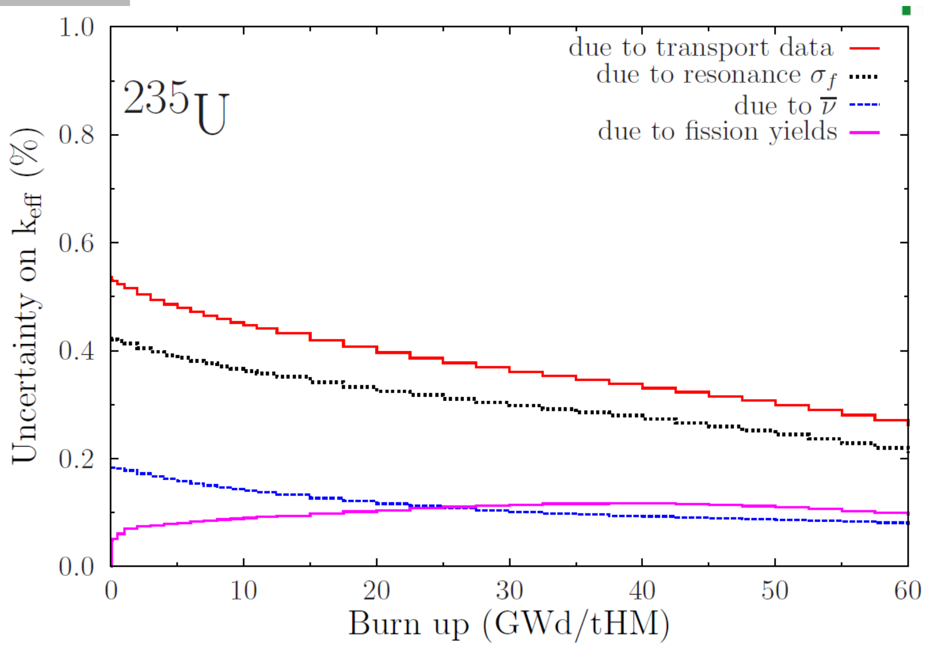
Results 3. Assembly

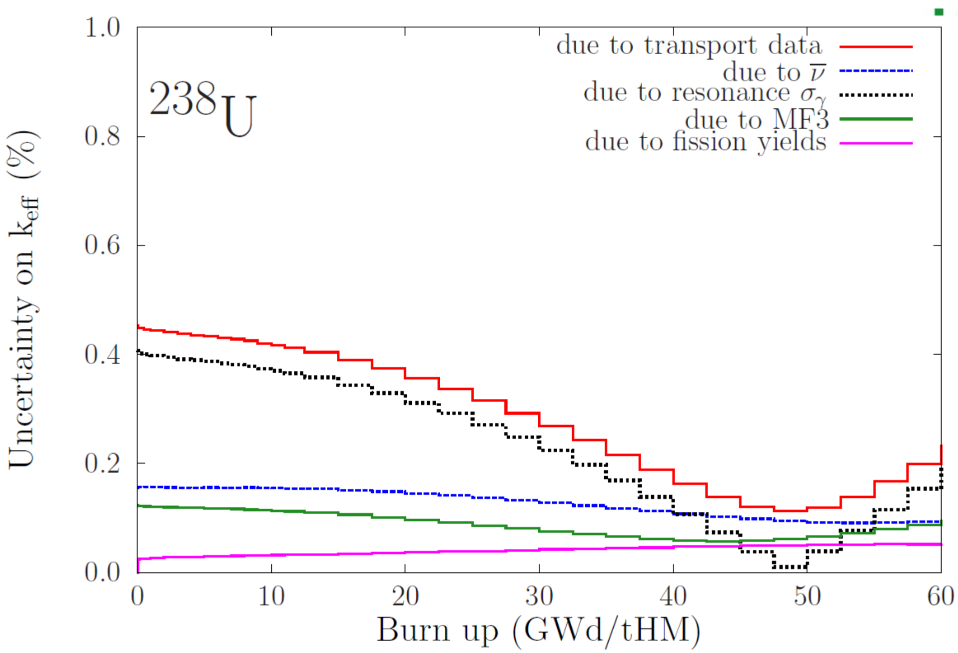
- K_{inf} uncertainty for 4 assemblies, 1 reactor cycle



Results 3. Assembly

- K_{inf} uncertainty contributions





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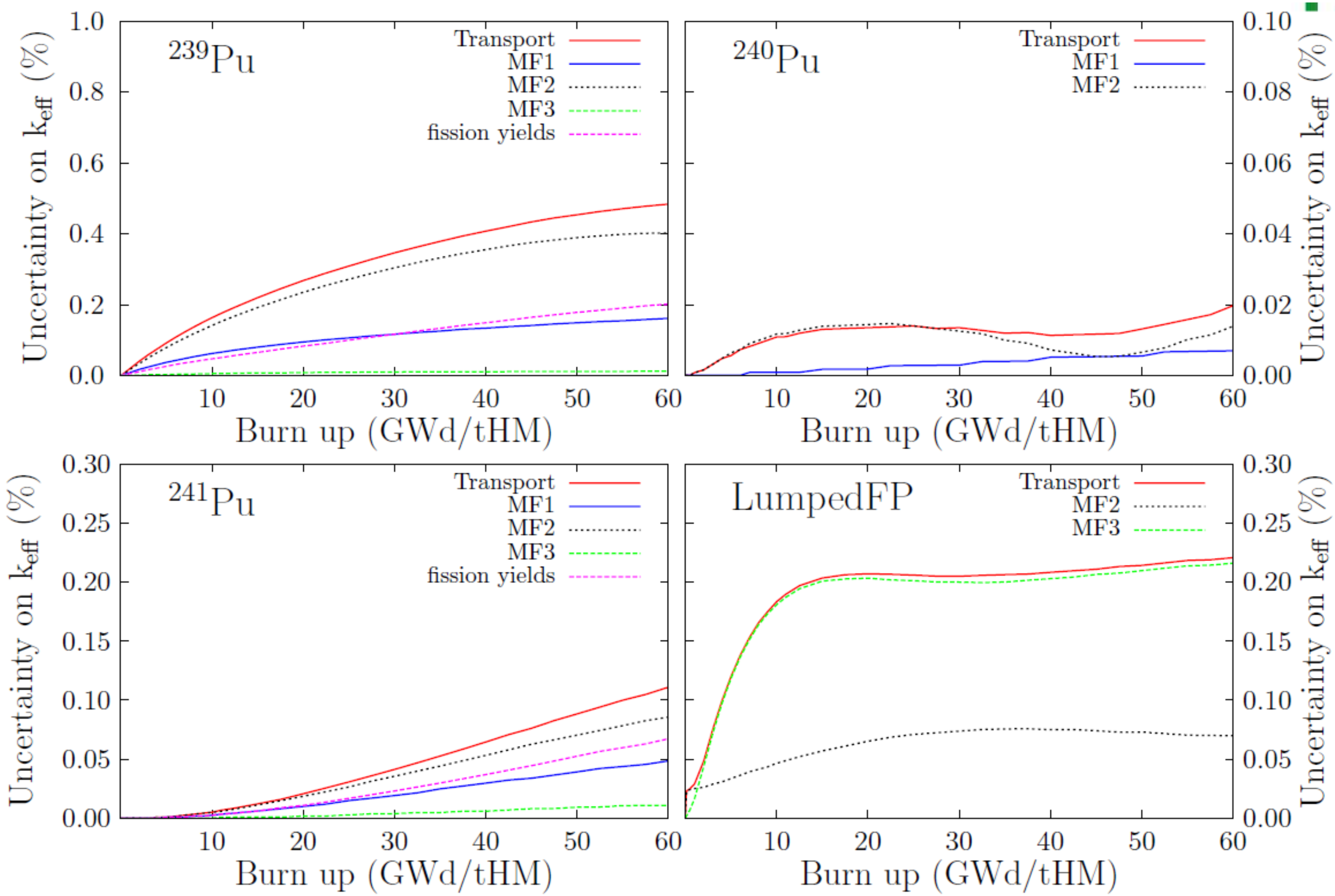
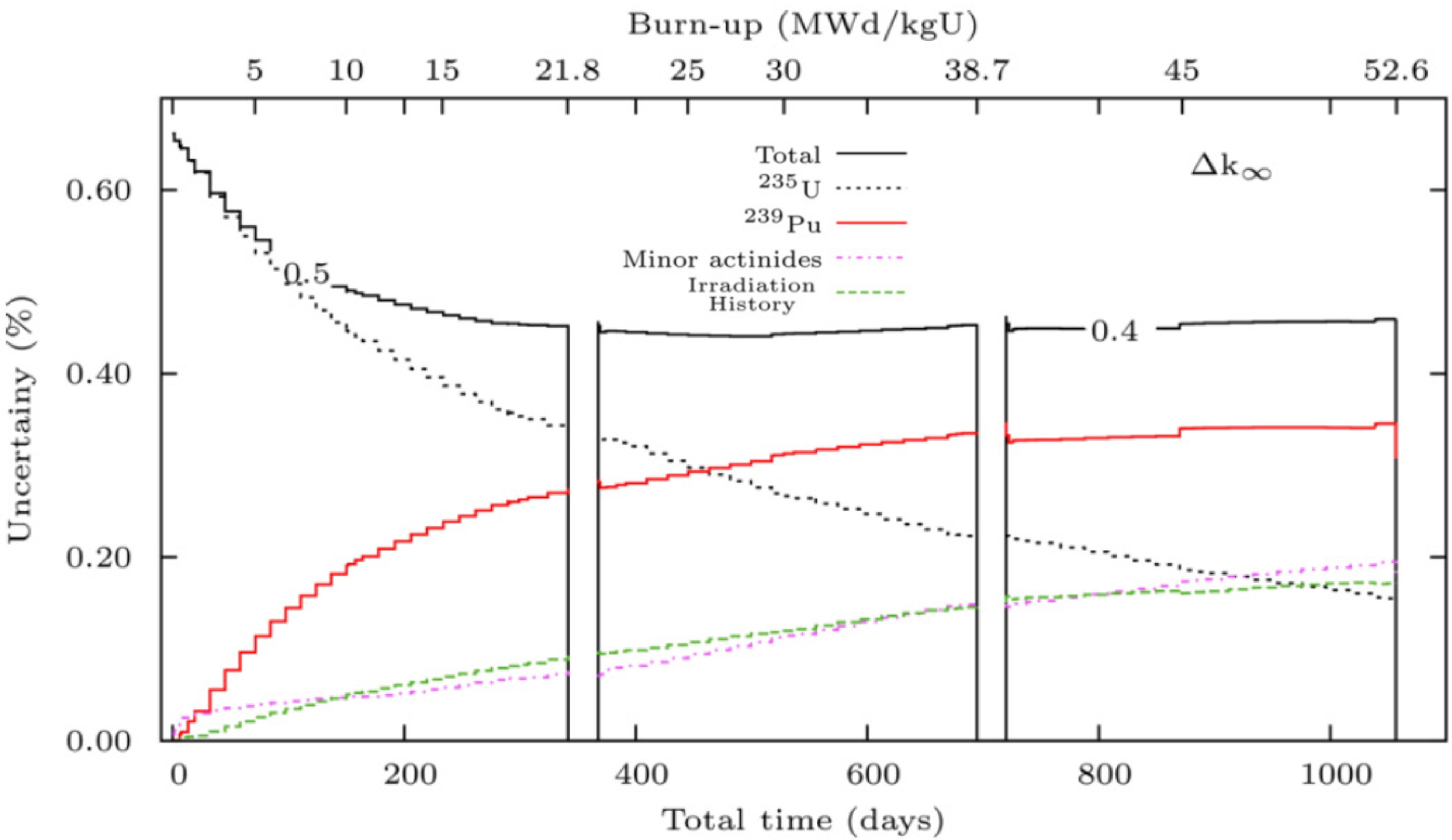
Results 3. Assembly

- K_{inf} uncertainty contributions



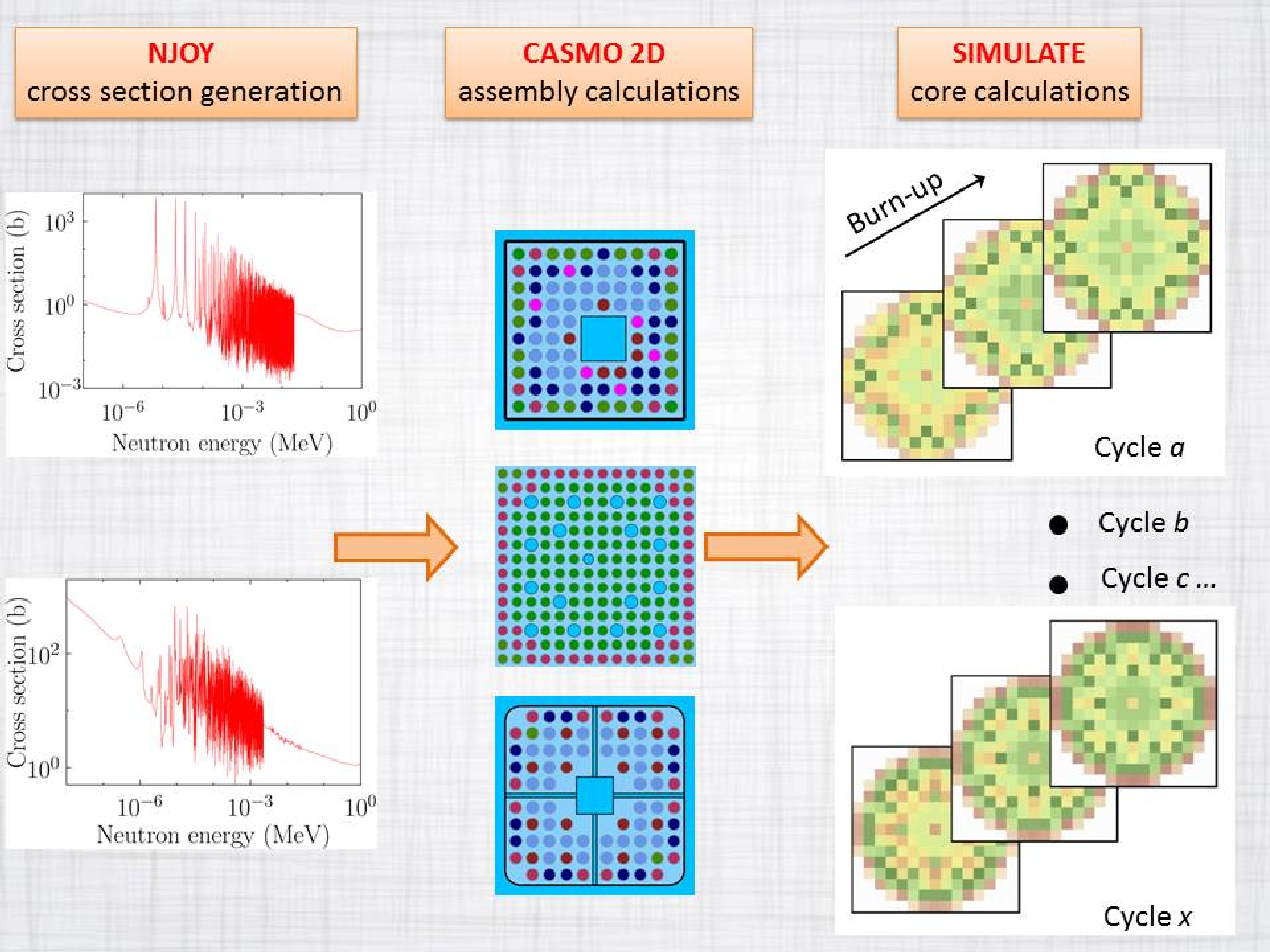
Results 3. Assembly

- K_{inf} uncertainty for a PWR UO_2, over 3 successive reactor cycles



Results 4. Full core

- Example with CASMO/SIMULATE,



Results 4. Full core

- Example with CASMO/SIMULATE,

Mean
Std (%)

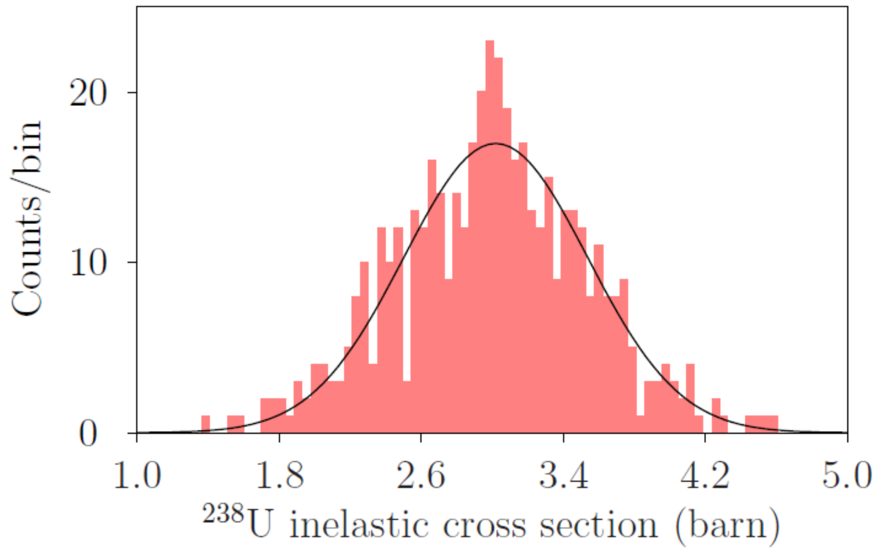
	1	2	3	4	5	6	7	8	9	10	11	12	13
A						0.35 0.6	0.43 0.4	0.35 0.6					
B				0.41 0.4	0.68 0.3	1.22 1.0	1.33 1.0	1.22 1.0	0.68 0.3	0.41 0.4			
C			0.46 0.5	1.23 0.9	1.28 0.4	0.97 0.3	0.92 0.6	0.98 0.5	1.29 0.4	1.23 0.9	0.46 0.5		
D		0.41 0.4	1.23 0.9	1.08 0.1	1.13 0.4	1.40 0.2	1.10 0.6	1.40 0.2	1.13 0.4	1.08 0.2	1.23 0.9	0.41 0.4	
E		0.68 0.3	1.29 0.4	1.13 0.4	1.28 0.4	1.30 0.5	1.26 0.6	1.30 0.5	1.28 0.4	1.13 0.4	1.28 0.4	0.68 0.3	
F	0.35 0.6	1.22 1.0	0.98 0.5	1.40 0.2	1.31 0.5	1.22 0.6	1.02 1.0	1.22 0.6	1.30 0.5	1.40 0.2	0.97 0.3	1.22 1.0	0.35 0.6
G	0.43 0.4	1.33 1.0	0.92 0.6	1.10 0.6	1.26 0.6	1.02 1.0	0.79 1.3	1.02 1.0	1.26 0.6	1.10 0.6	0.92 0.6	1.33 1.0	0.43 0.4
H	0.35 0.6	1.22 1.0	0.97 0.3	1.40 0.2	1.30 0.5	1.22 0.6	1.02 1.0	1.22 0.6	1.30 0.5	1.40 0.2	0.98 0.5	1.22 1.0	0.35 0.6
I		0.68 0.3	1.28 0.4	1.13 0.4	1.28 0.4	1.31 0.5	1.26 0.6	1.30 0.5	1.28 0.4	1.13 0.4	1.29 0.4	0.68 0.3	
J		0.41 0.4	1.23 0.9	1.07 0.2	1.13 0.4	1.40 0.2	1.10 0.6	1.40 0.2	1.13 0.4	1.07 0.2	1.23 0.9	0.41 0.4	
K			0.46 0.5	1.23 0.9	1.29 0.4	0.98 0.5	0.92 0.6	0.97 0.3	1.28 0.4	1.23 0.9	0.46 0.5		
L				0.41 0.4	0.68 0.3	1.22 1.0	1.33 1.0	1.22 1.0	0.68 0.3	0.41 0.4			
M						0.35 0.6	0.43 0.4	0.35 0.6					

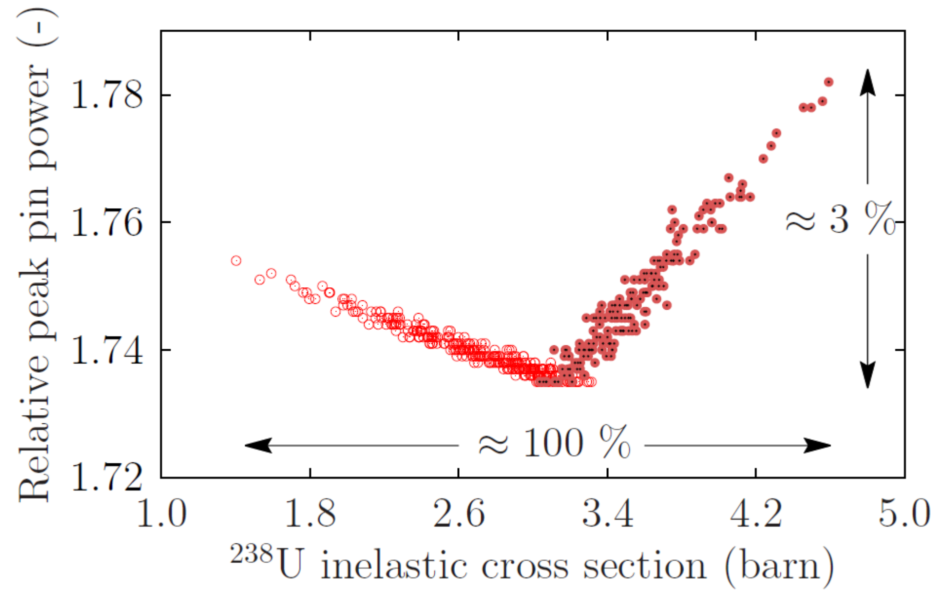
Rel. Std.
max 1.35%
min 0.15%
mean 0.54%

Relative radial power distributions of the UO_2

4. Full core: Important core parameter: peak pin power

- Consequence for the ppp (peak pin power), cycle 6, 7 days after the start of a specific reactor:



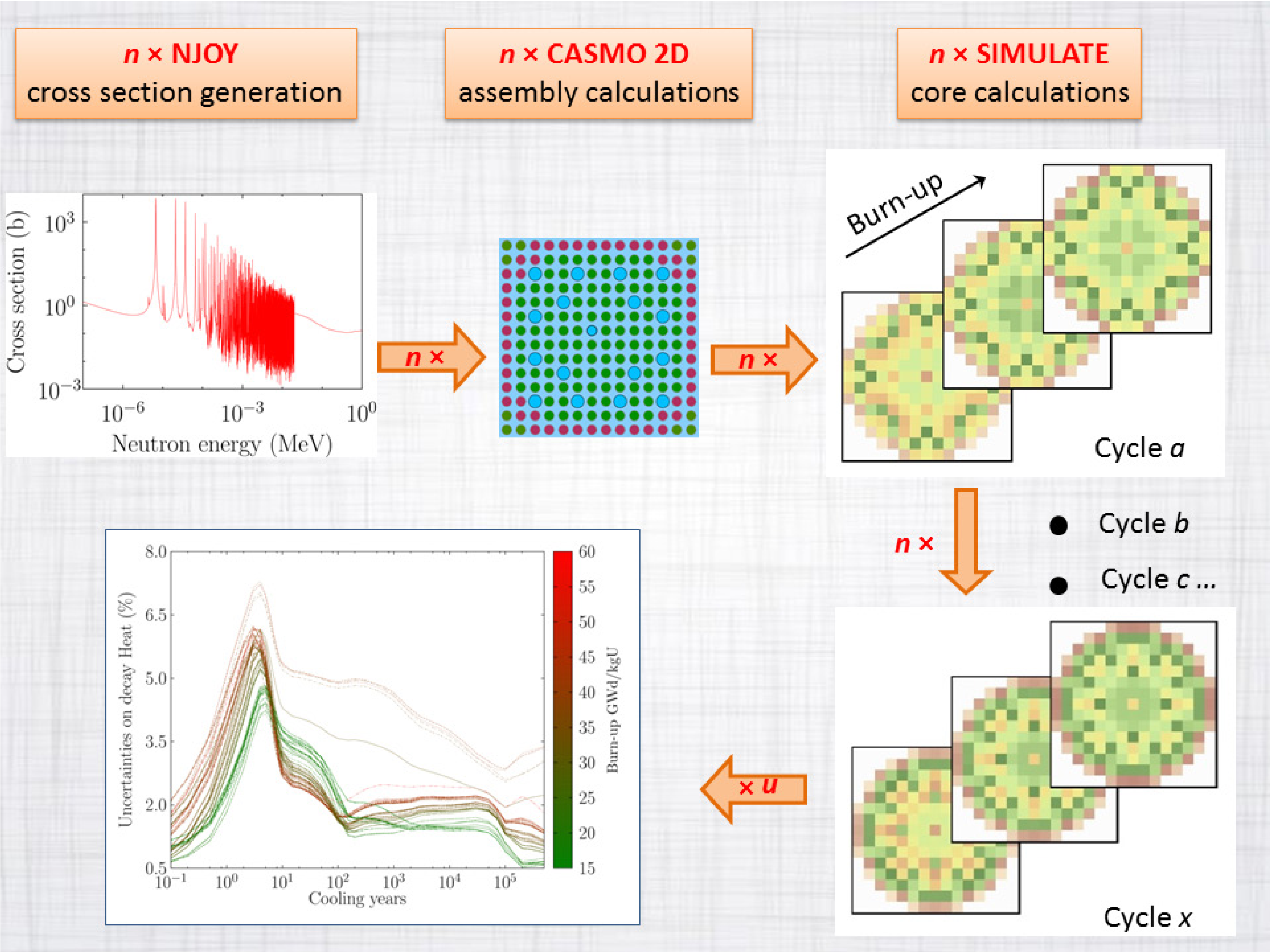


- Strong nonlinearity due to ^{238}U(n,inl), combined with spatial effect.
- Decreasing part: ppp at the core center,
- Increasing part: ppp at the core side.
- To be avoided in core licensing: strong skewness, non Gaussian (sensitivity method will miss it)

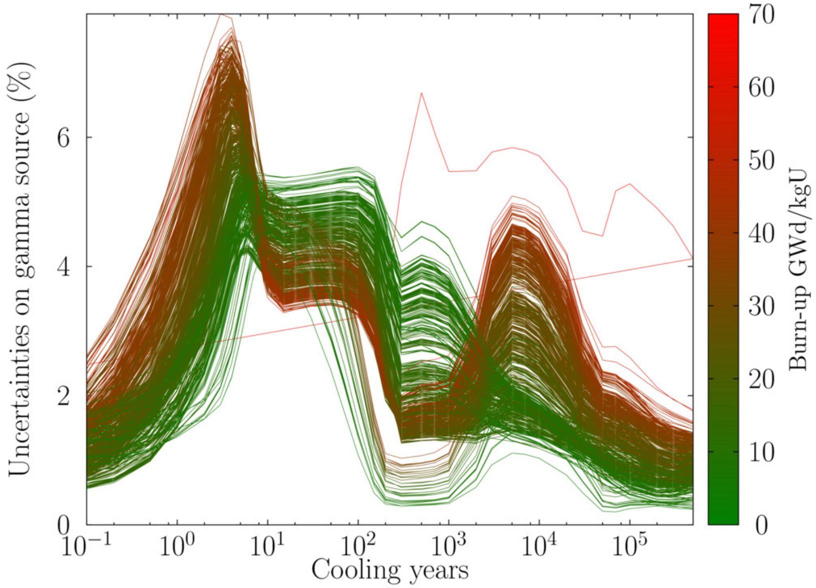
- Only possible because of the high uncertainty on ^{238}U(n,inl) (20% from 1 to 5 MeV)

Results 5. Spent fuel

- Total Monte Carlo approach: random nuclear data for the full calculation chain.



Results 5. Spent fuel



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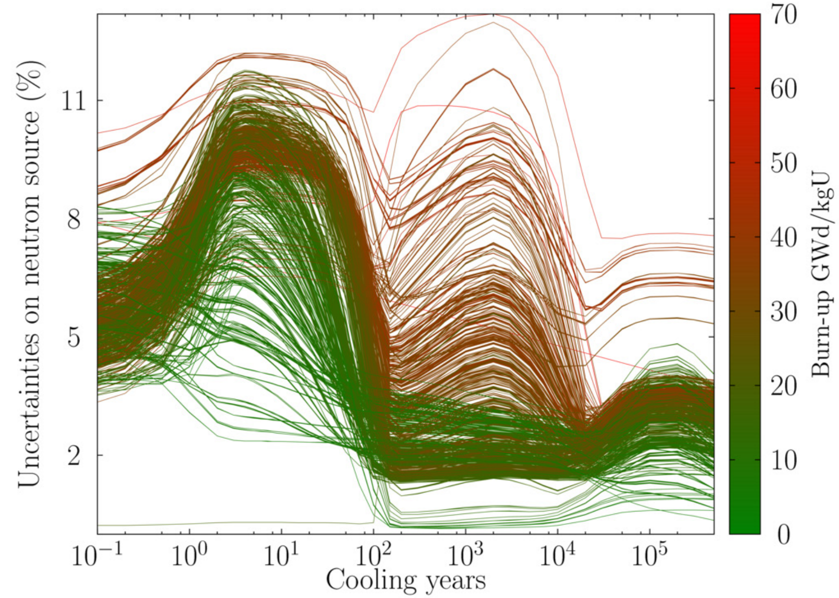
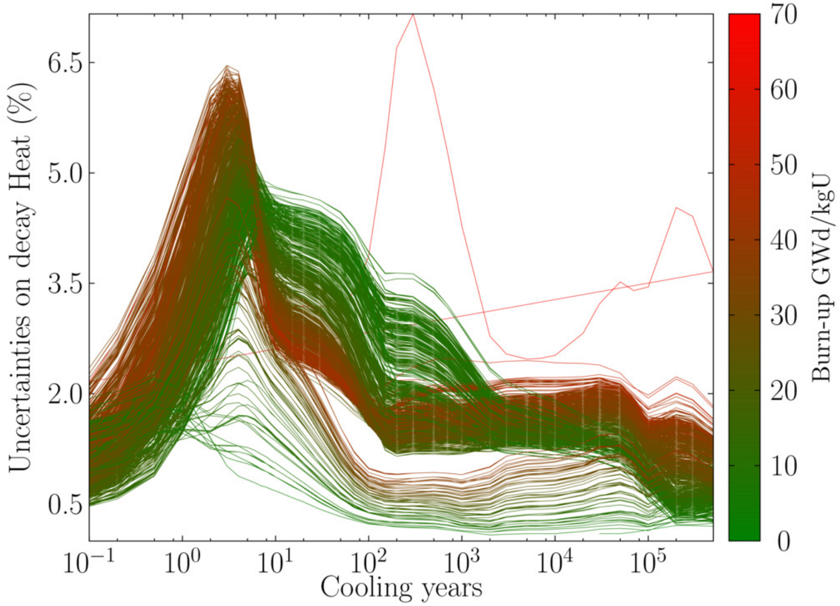
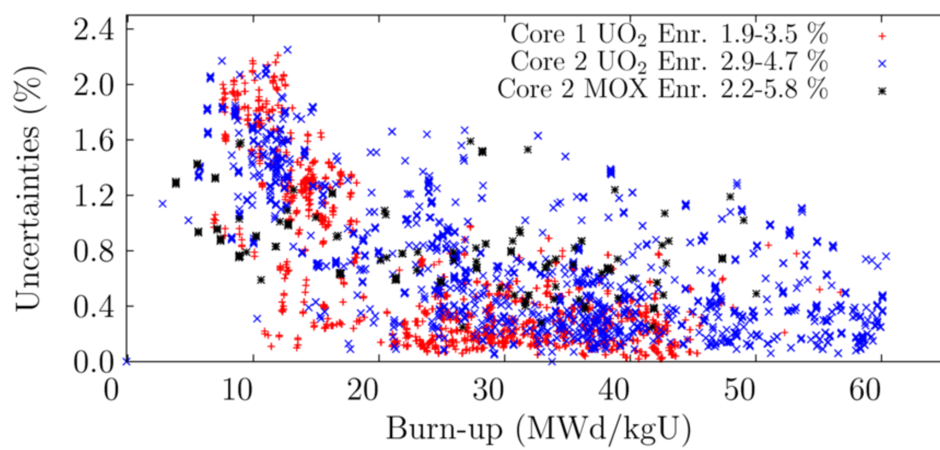






Results 6. Transient

- Control Rod Ejection Accident, with ND uncertainties ($^{235,238}U$, ^{239}Pu, thermal scattering)

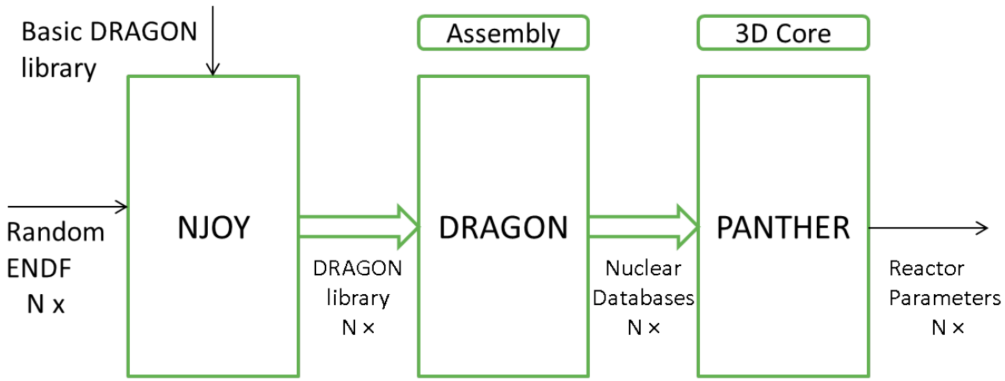


Figure 1. Calculation scheme for the determination of the uncertainties in the main reactor parameters due to nuclear data uncertainties.

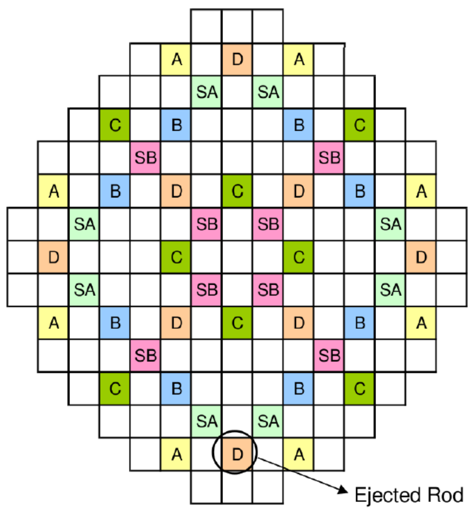
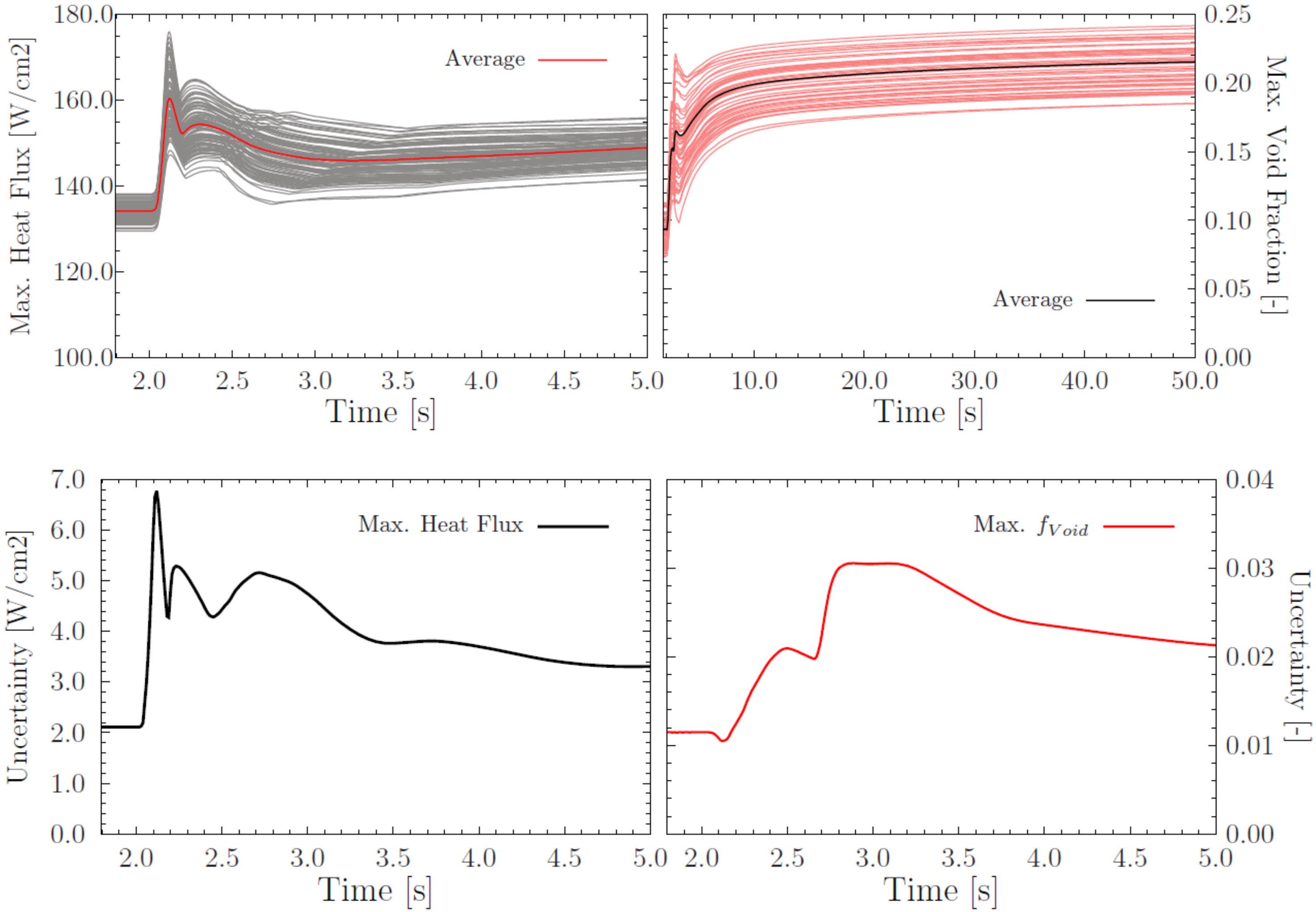


Figure 2. Scheme of Westinghouse core with distribution of control rod banks and position of the ejected control rod.

Results 6. Transient

- Control Rod Ejection Accident, with ND uncertainties



Uncertainty from methods

"Among different participants, given a model definition, which uncertainties do we obtain ?

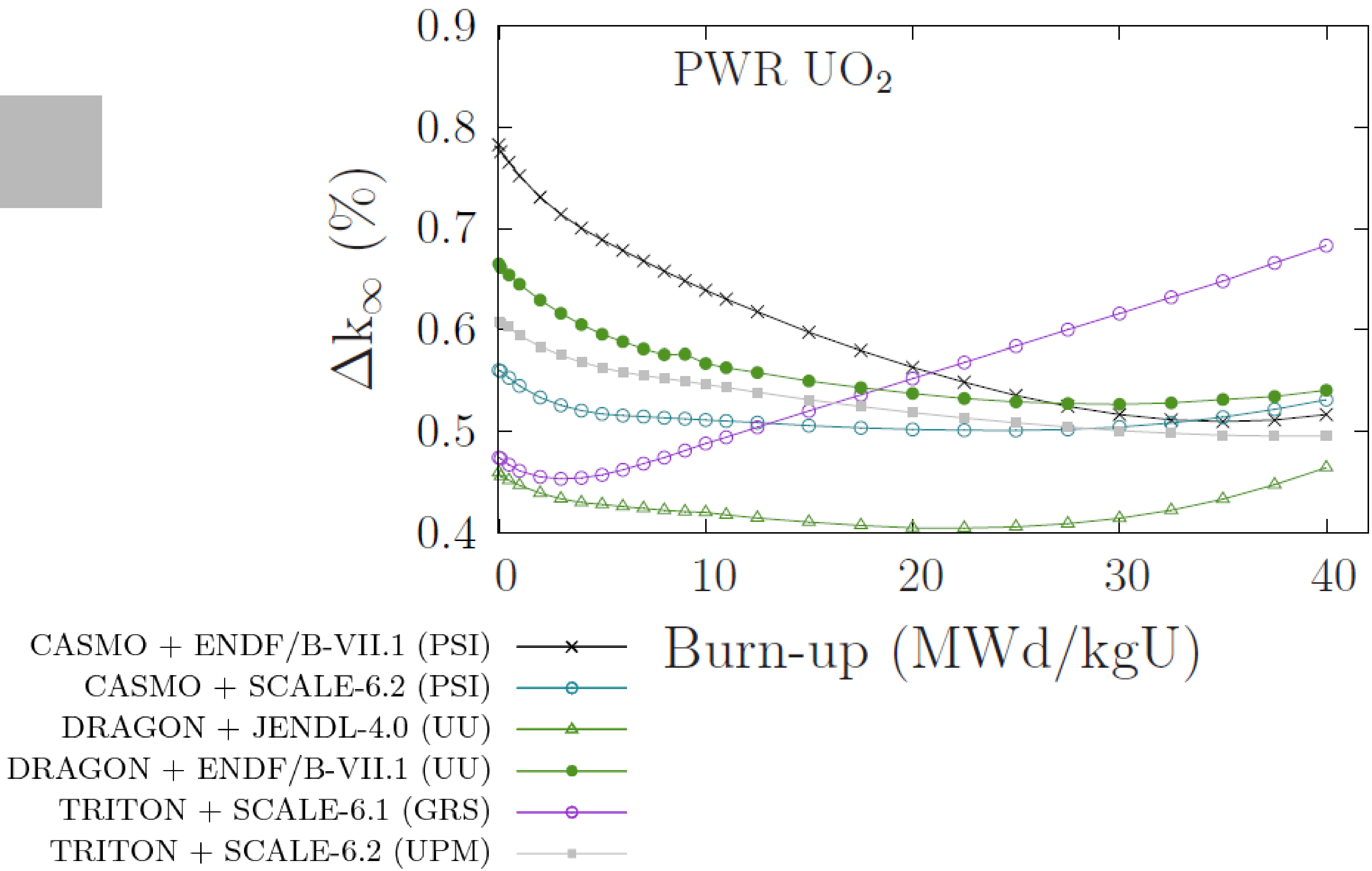
How are the spread of uncertainties compared to the uncertainties themselves ?"

- Uncertainties due to nuclear data are larger than from many other sources,

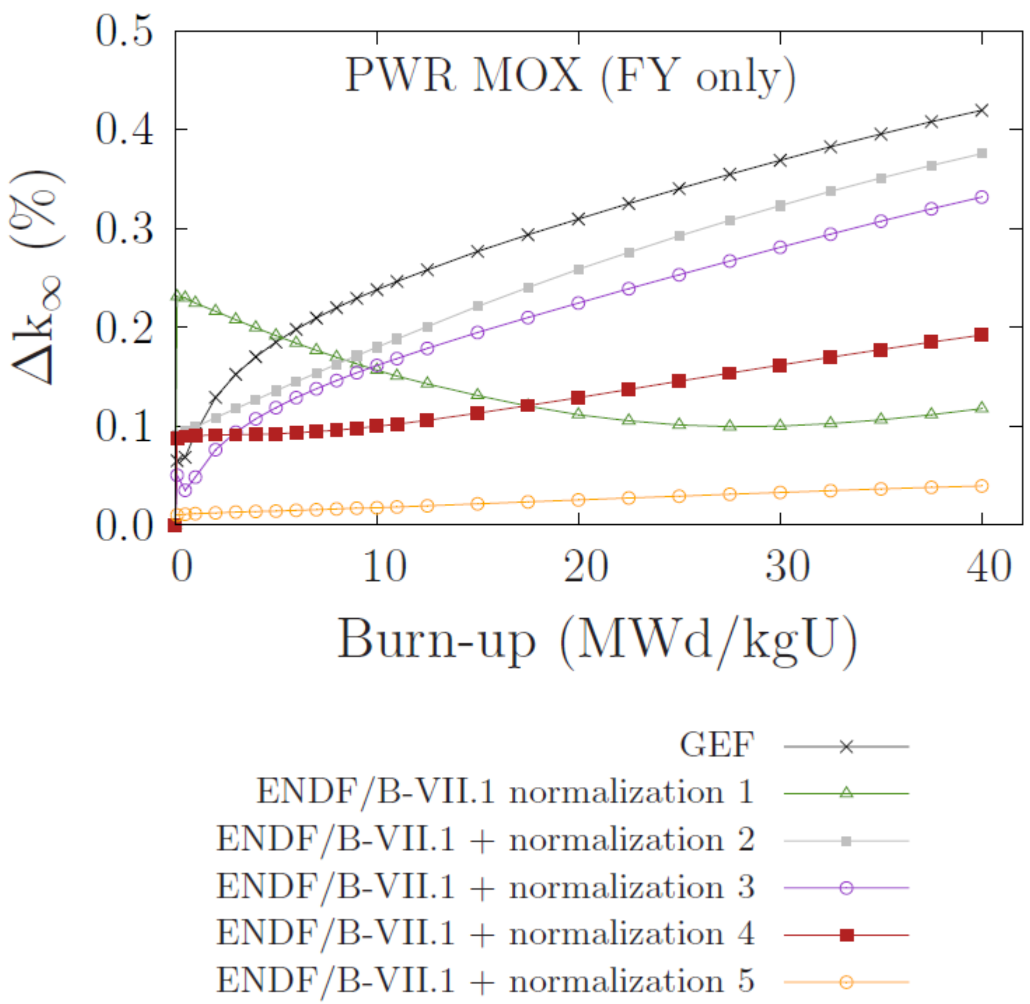
1. Sources of nuclear data uncertainties vary: JEFF, ENDF/B, JENDL,TENDL,SCALE, in-house…
2. Processing of nuclear data vary,
3. Methods of uncertainty propagation vary: deterministic, Monte Carlo,
4. Methods of neutron transport/depletion also vary.

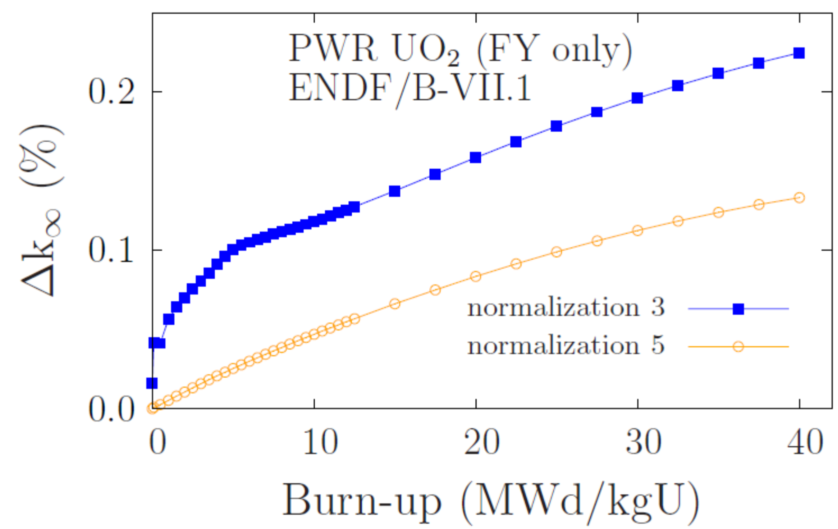
- This approach is then different than the UAM requirements,
- It is close to a real-case assignment given by a third party to a TSO (Technical Support Organization).

Uncertainty from methods



Uncertainty from methods





Normalization 1:	mass & charge
Normalization 2:	GEF correlation
Normalization 3:	Updated GEF (see [1])
Normalization 4:	∑FY=2
Normalization 5:	SANDY

Other Uncertainties

- For assembly/reactor calculations, other sources of uncertainties appear:
  - Nuclear data,
  - Reactor operating conditions,
  - Manufacturing tolerances,
  - Burnup induced technological changed,
  - …
- All play a role for the assessment on the final quantities

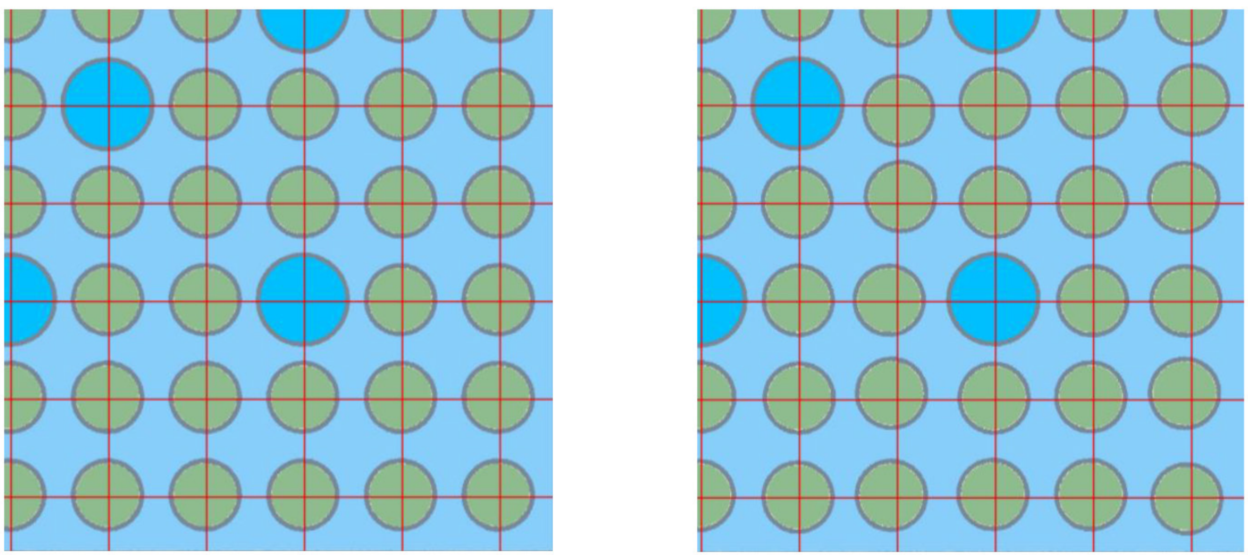
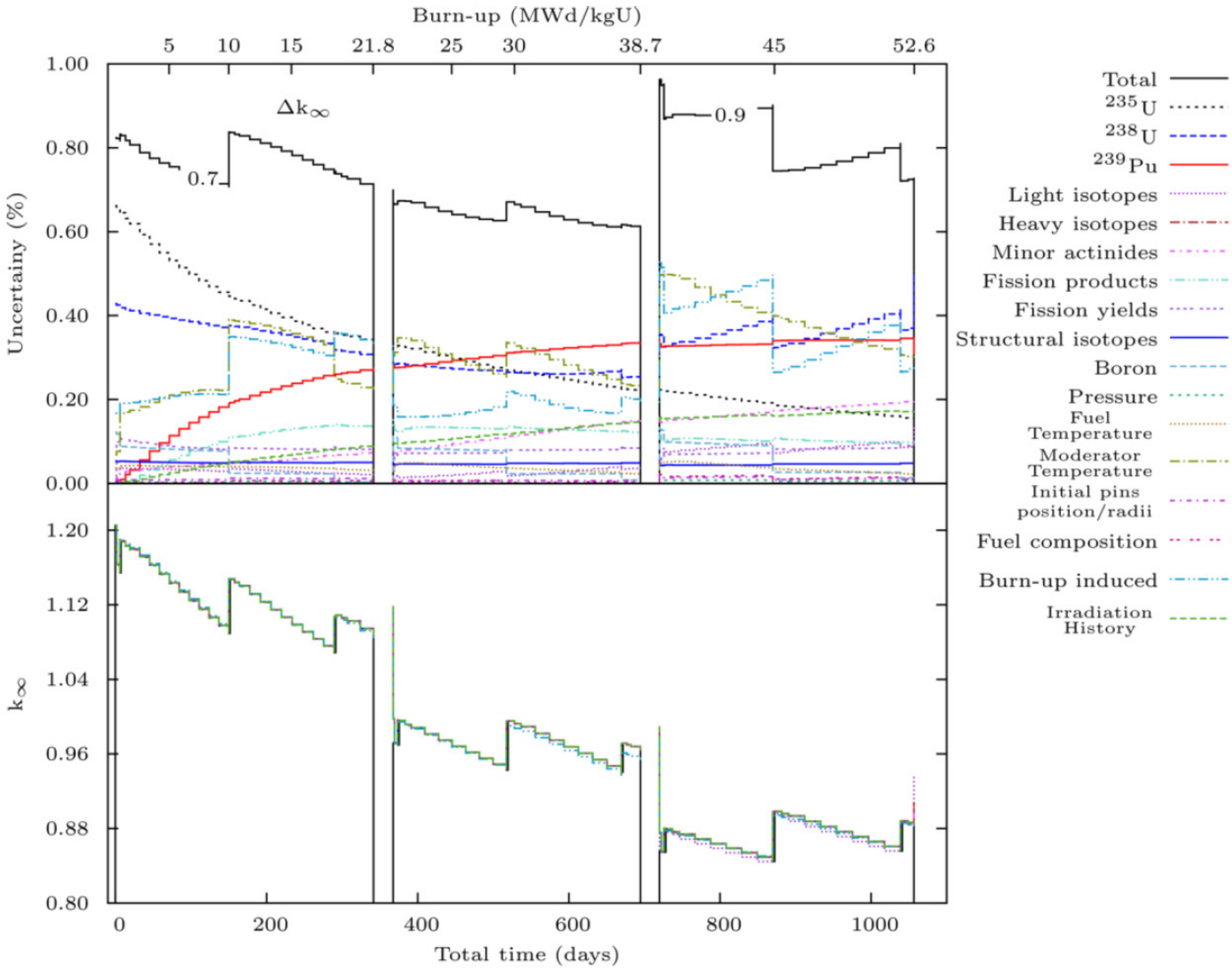


Figure 9: Two random distributions of fuel pins with different enrichments and densities. The colors indicate different fuel pins.

Other Uncertainties



Conclusion

1. Nuclear data uncertainties can nowadays be propagated in large-scale systems, to any quantities

2. A necessary condition is to be able to randomly change the nuclear data (not possible if hardcoded in simulation codes).

3. Other sources of uncertainties exist

4. Finally, uncertainties should be replaced by pdf.

The spread of uncertainties can be higher than the uncertainties themselves (because of methods, sources of data, codes…).
This puts in perspective calculated uncertainties.

Wir schaffen Wissen – heute für morgen