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Nuclear data uncertainty quantification and propagation Nuclear data for power reactors and fuel

Joint ICTP-IAEA workshop, Trieste, Italy, October 10-12th, 2017

- General comments
 - Applications to energy systems
 - I. Methods: Monte Carlo (TMC) vs. perturbation (sensitivity)
 - II. Results with TMC
 1. Criticality-safety benchmarks
 2. PWR Fuel pin keff
 3. Assemblies
 4. Full core
 5. Transient
 6. Bowing effect
 7. Spent Nuclear Fuel
 8. Loading curves for final repository
 - III. Uncertainties from methods
 - IV. Other uncertainties
- All slides can be found here: https://tendl.web.psi.ch/bib_rochman/presentation.html

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 \Rightarrow safety \Rightarrow 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

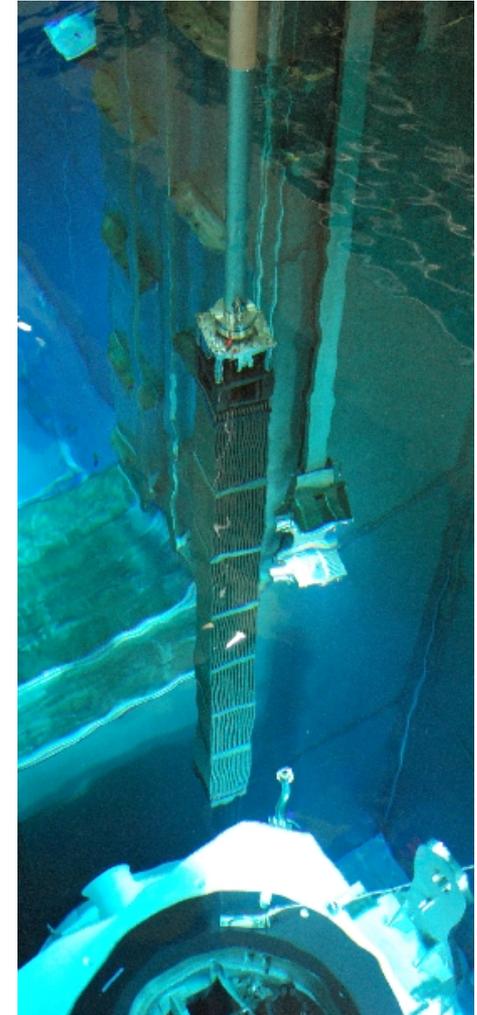
Are nuclear data important ?

In energy production, better nuclear data can help for:

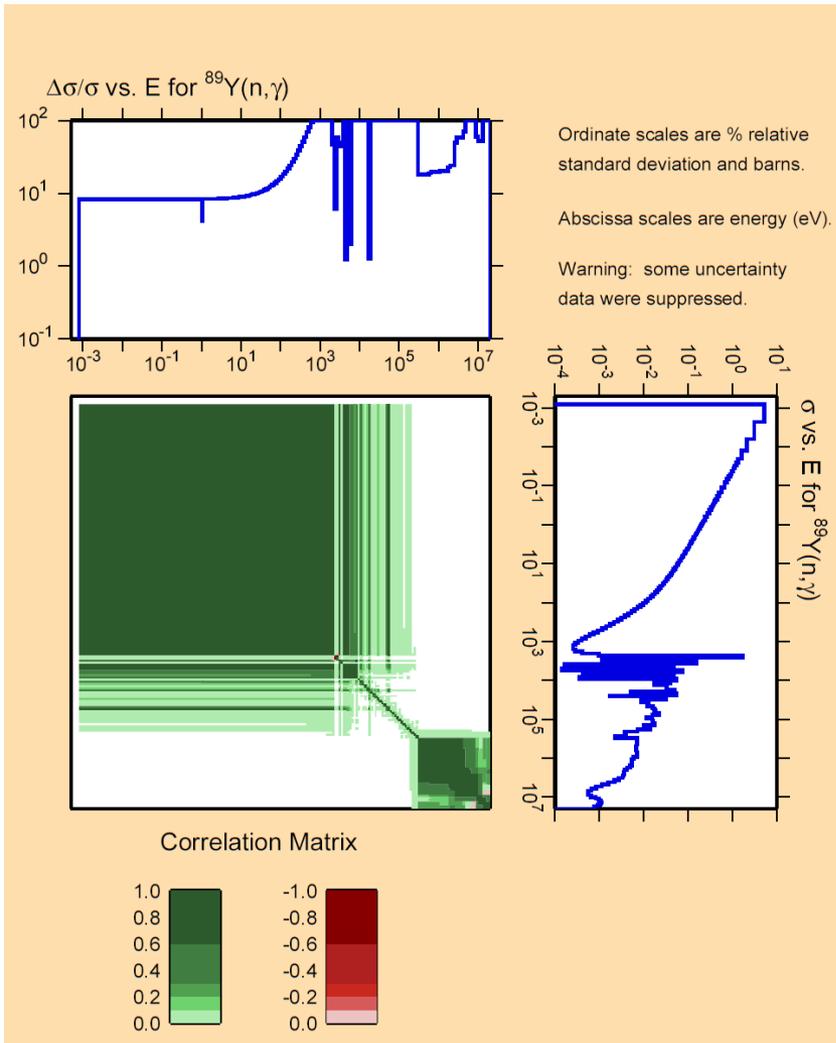
- Fuel storage and processing,
- Life-time extension,
- Outside usual reactor operations,
- Dosimetry,
- Higher fuel burn-up,
- cost reduction in design of new systems,
- Isotope production,
- Shielding (people safety),
- Future systems,

Better nuclear data have a limited effect on:

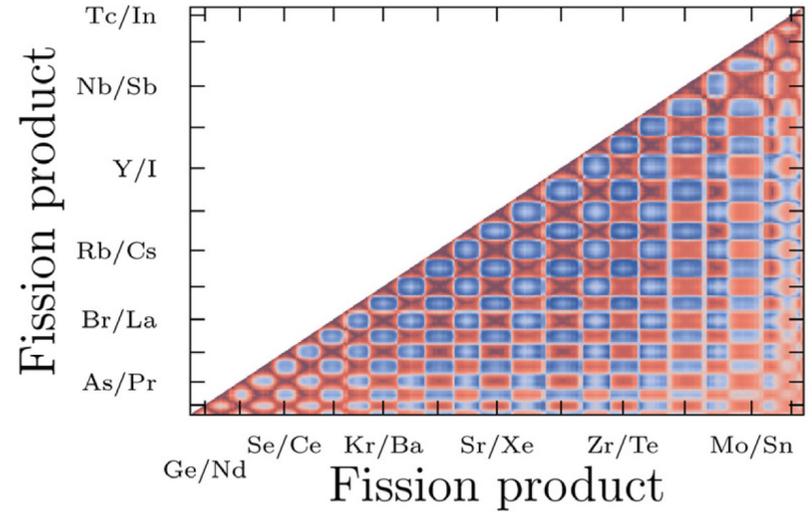
- Current reactor operation,
- Current reactor safety,
- Accident simulation,
- Proliferation,
- Chernobyl, TMI, Fukushima and other accident.



Nuclear data uncertainties: examples



$^{89}\text{Y}(n,g)$



Three methods exist today:

1. Based on nuclear data covariance data

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

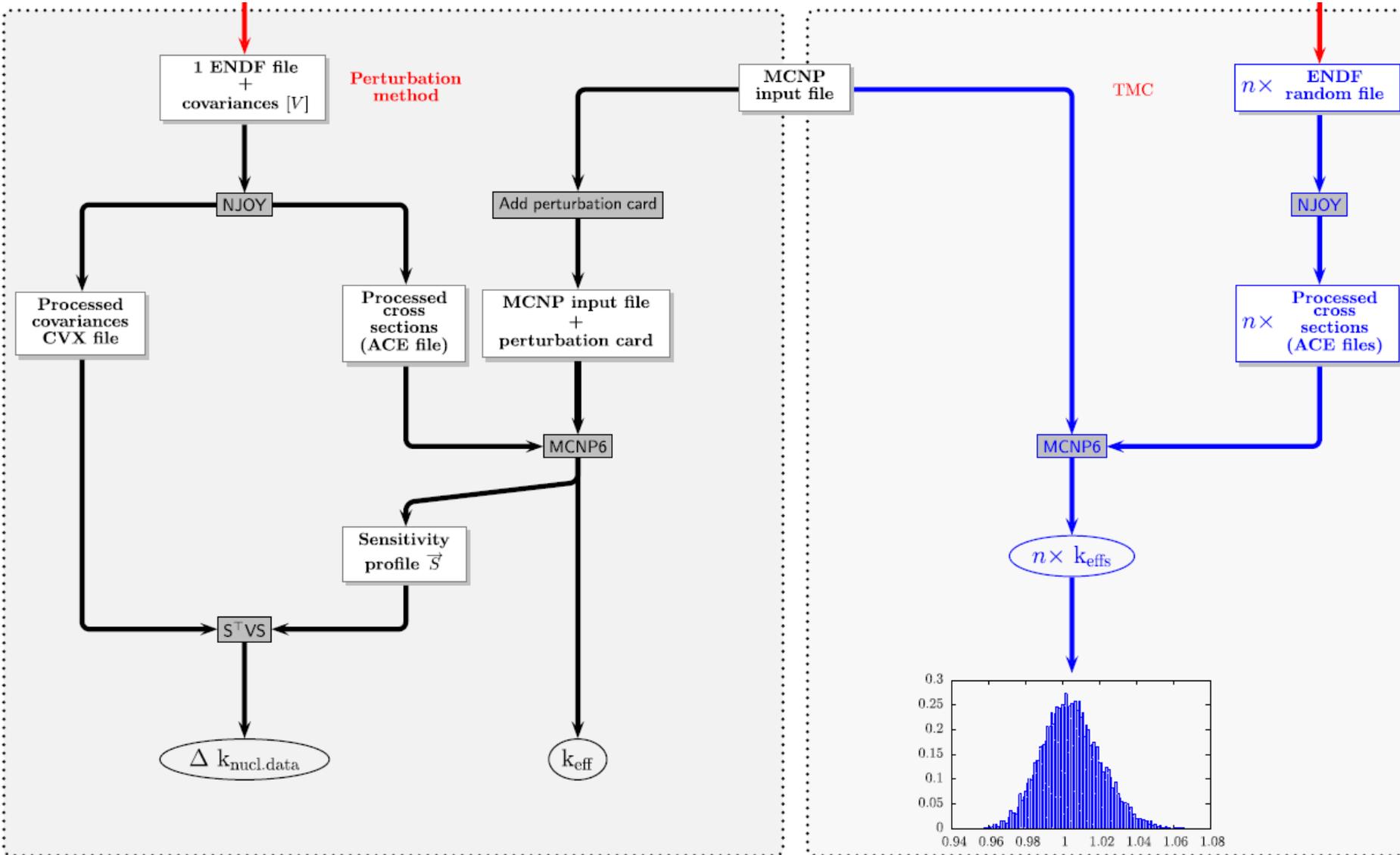
2. Based on nuclear data parameter covariance data:

- So-called TMC (Total Monte Carlo)
- 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...

- As mentioned before, there are basically two ways of propagating uncertainties



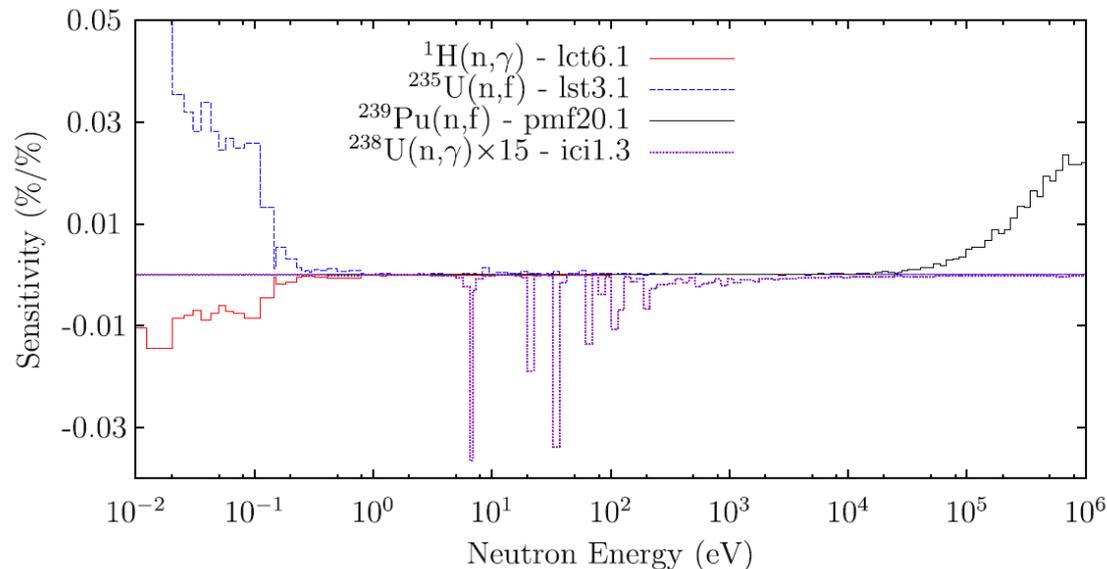
Uncertainty propagation: Sandwich rule

$$\sigma_R^2 = \sum_{ij} S_i^R C(\alpha_i \alpha_j) S_j^R = \vec{S} C \vec{S}^T, \quad (1)$$

Eq. (1) succinctly summarizes the information required to calculate the relative variance ($\sigma_R^2 = \left(\frac{\delta R}{R}\right)^2$) of a linearized system response R as the product of the relative sensitivity coefficient \vec{S} and the relative covariance matrix C of inputs (α_i), $i = 1, \dots, N$, where

$$\vec{S} = (S_1^R, \dots, S_N^R); S_i^R = \frac{\partial R}{R} \frac{\alpha_i}{\partial \alpha_i};$$

$$C(\alpha_i \alpha_j) = \frac{\text{COV}(\alpha_i \alpha_j)}{\alpha_i \alpha_j}. \quad (2)$$



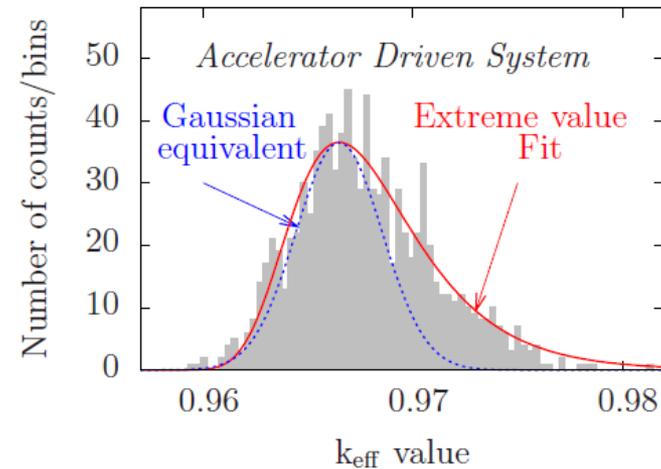
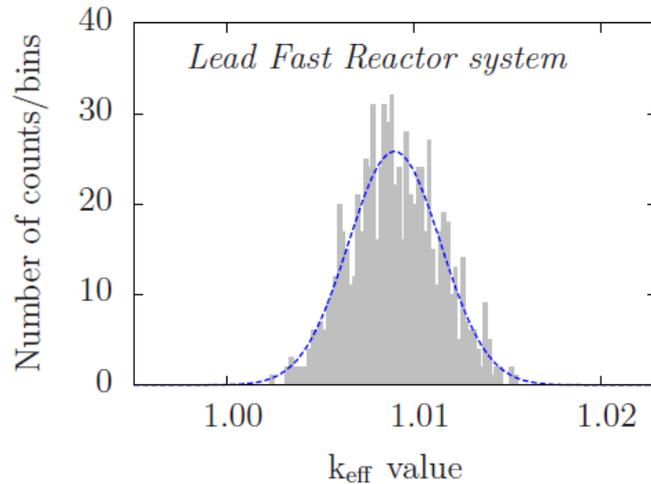
Uncertainty propagation: TMC

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.

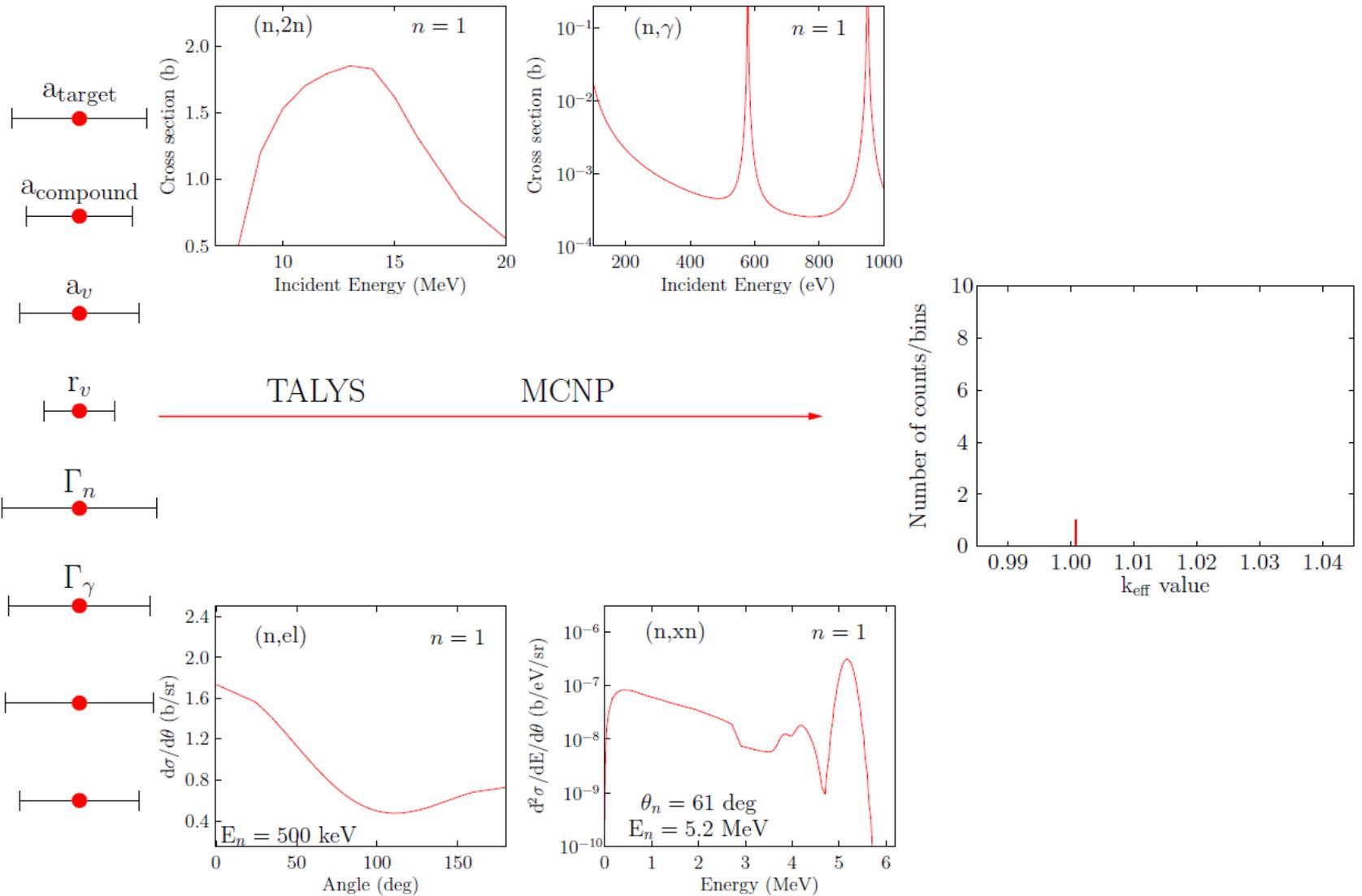
$$\sigma_{\text{total}}^2 = \sigma_{\text{statistics}}^2 + \sigma_{\text{nuclear data}}^2$$



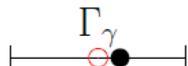
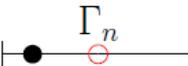
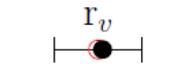
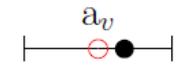
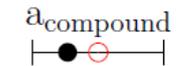
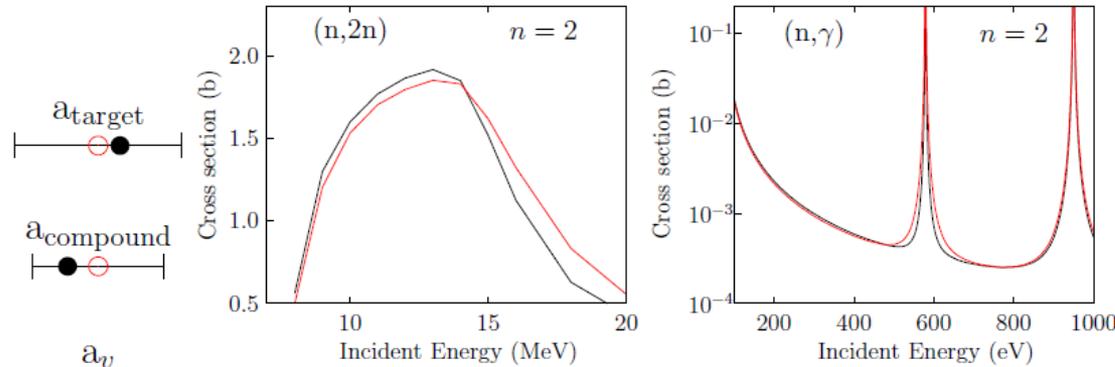
”Towards sustainable nuclear energy: Putting nuclear physics to work”,

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

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

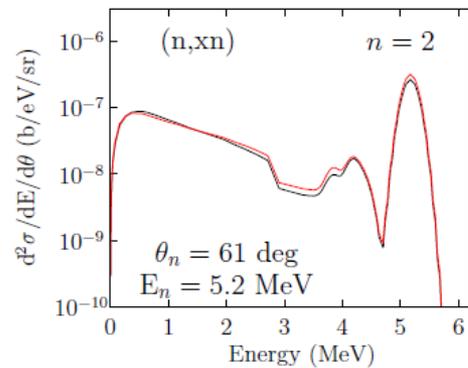
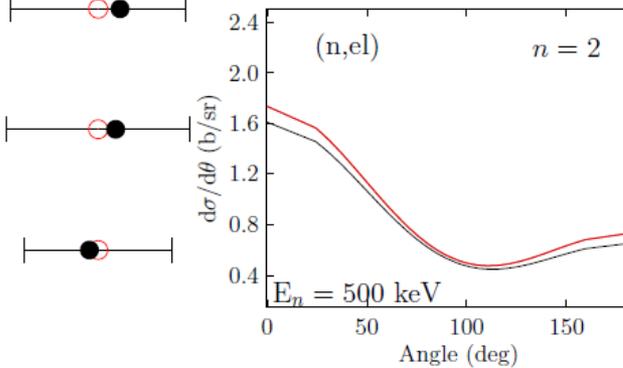
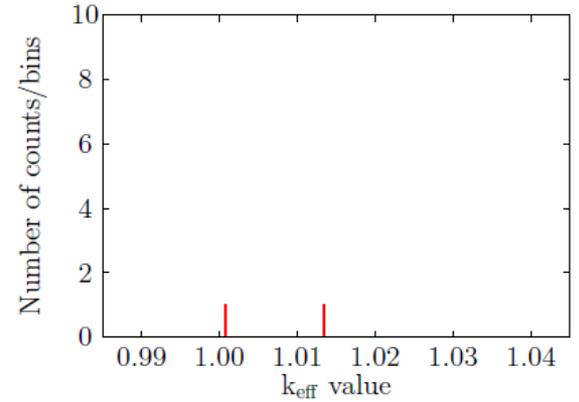


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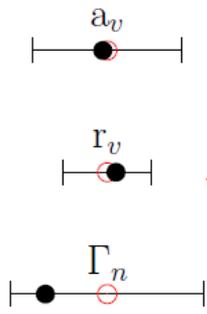
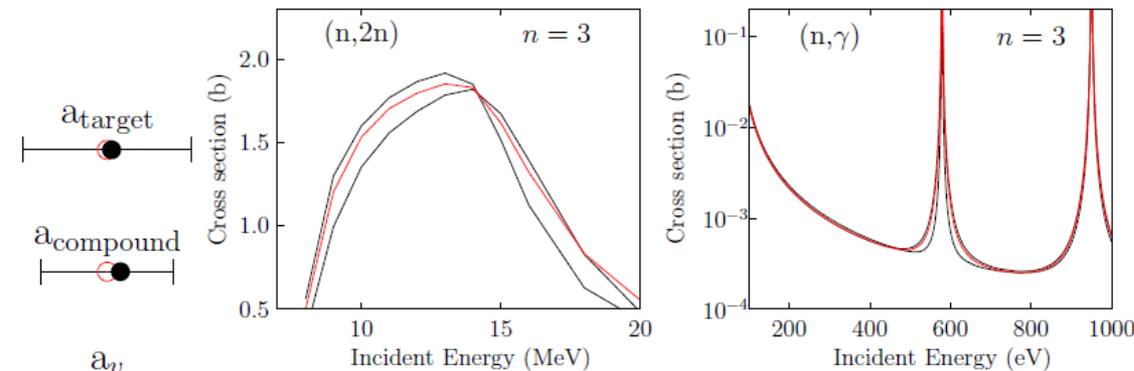


TALYS

MCNP

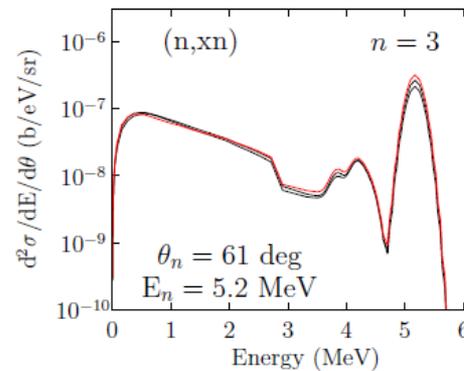
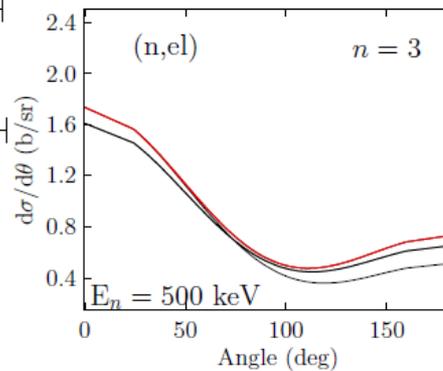
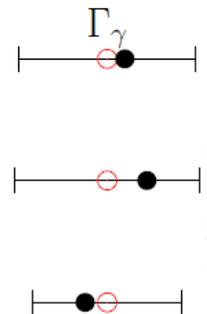
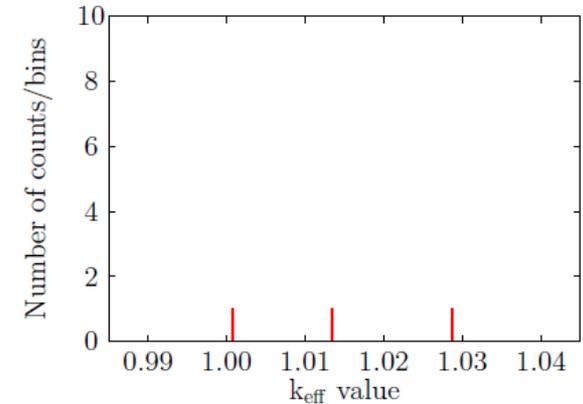


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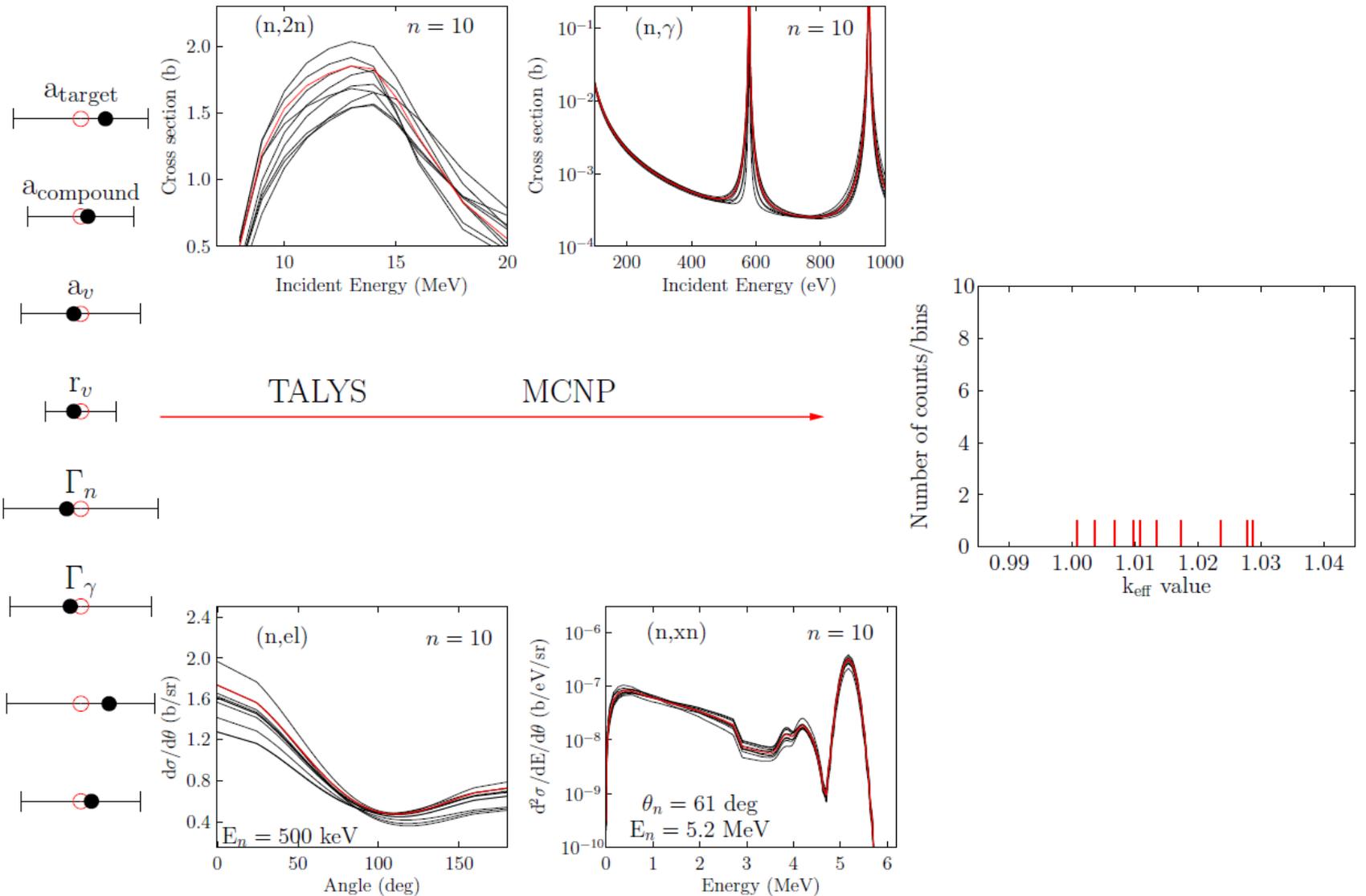


TALYS

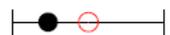
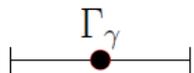
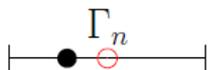
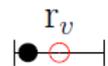
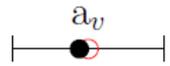
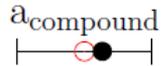
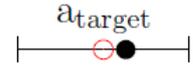
MCNP



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



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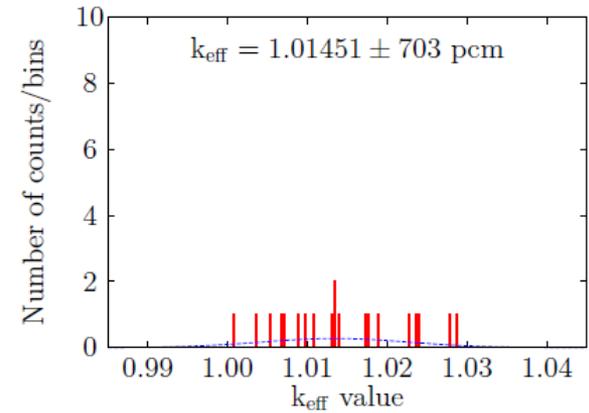


TALYS

MCNP

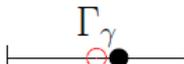
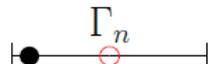
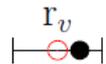
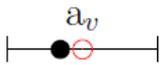
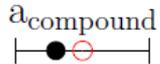
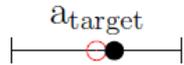


$n = 20$





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

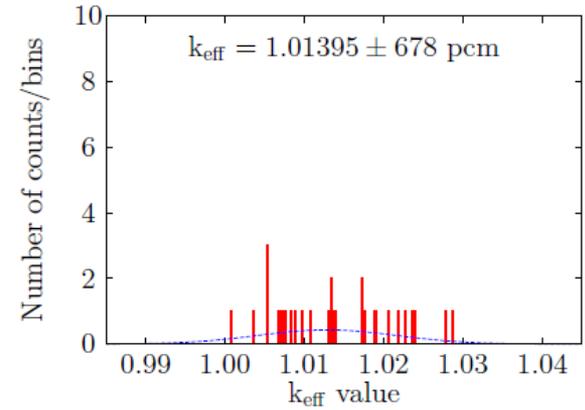


TALYS

MCNP

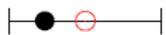
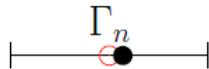
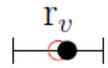
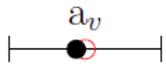
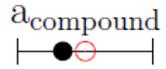
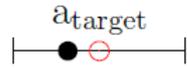


$n = 30$





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

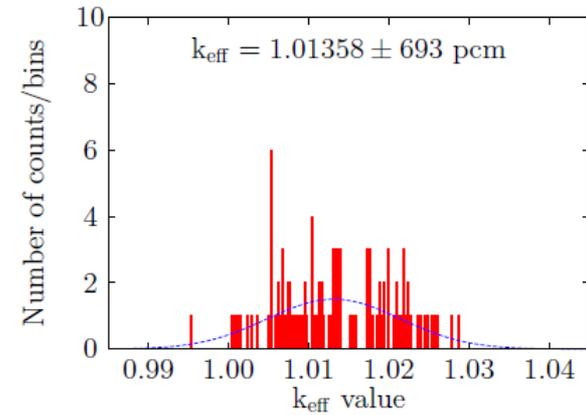


TALYS

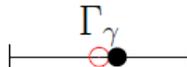
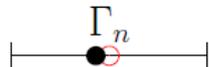
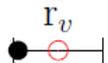
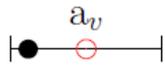
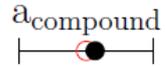
MCNP



$n = 100$

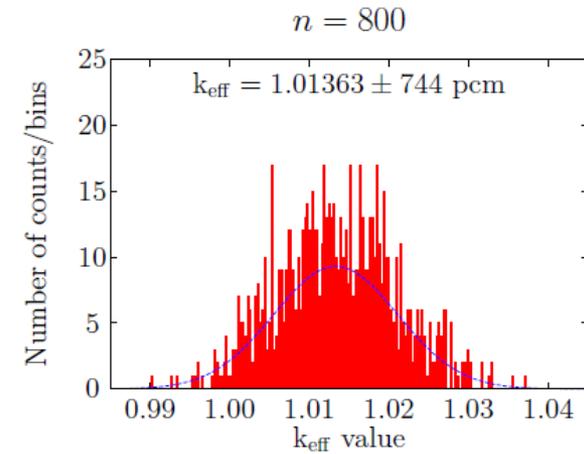


Hands on “1000 × (TALYS + ENDF + NJOY + MCNP) calculations”

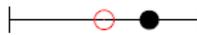
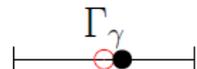
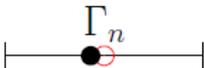
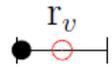
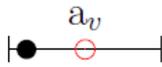
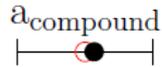
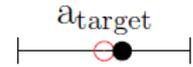


TALYS

MCNP

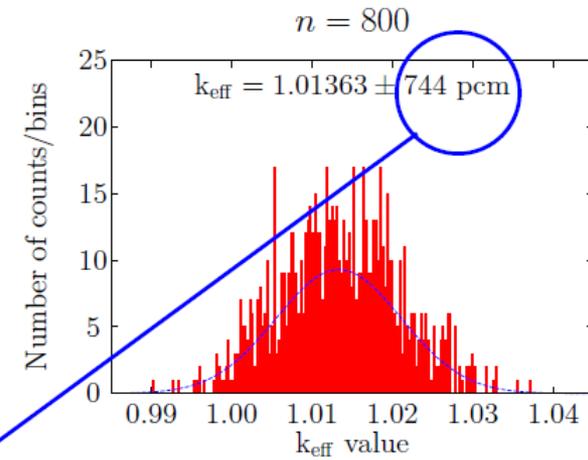


Hands on “1000 × (TALYS + ENDF + NJOY + MCNP) calculations”



TALYS

MCNP



Statistical uncertainty $\simeq 68$ pcm
 \implies uncertainty due to nuclear data $\simeq 740$ pcm

- In any case, uncertainties are not real quantities, contrary to cross sections
- They are only a reflection of the method applied and of the considered inputs !

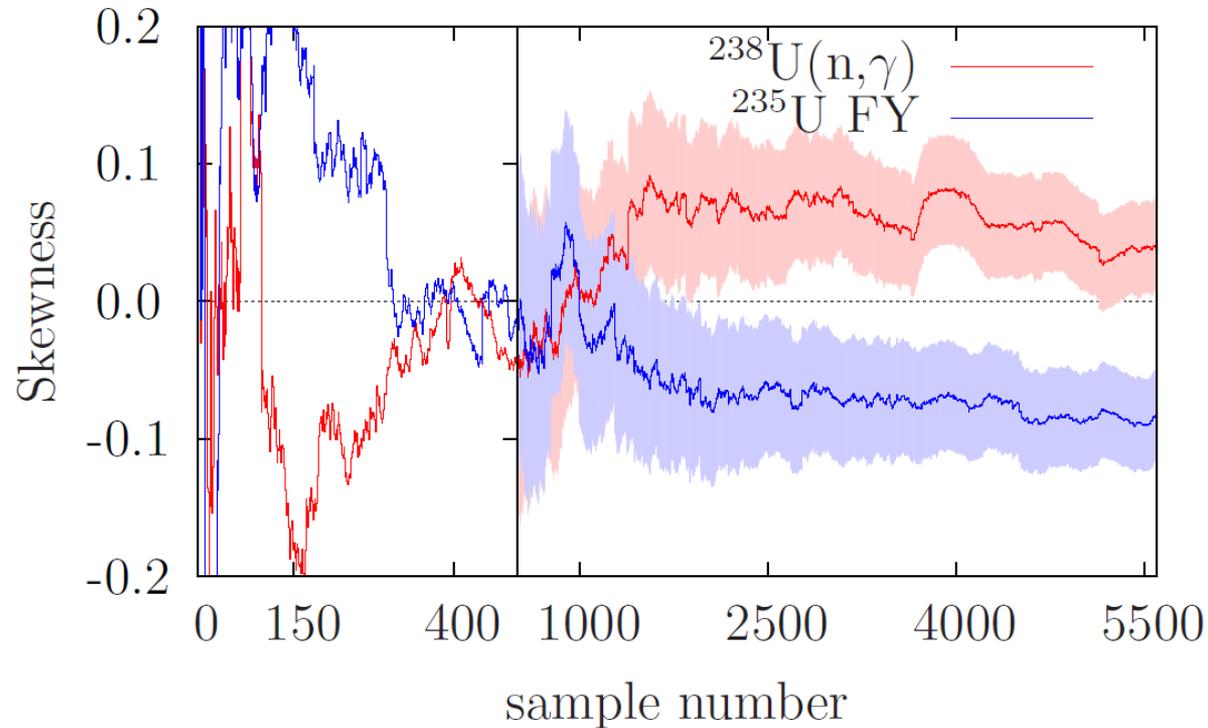
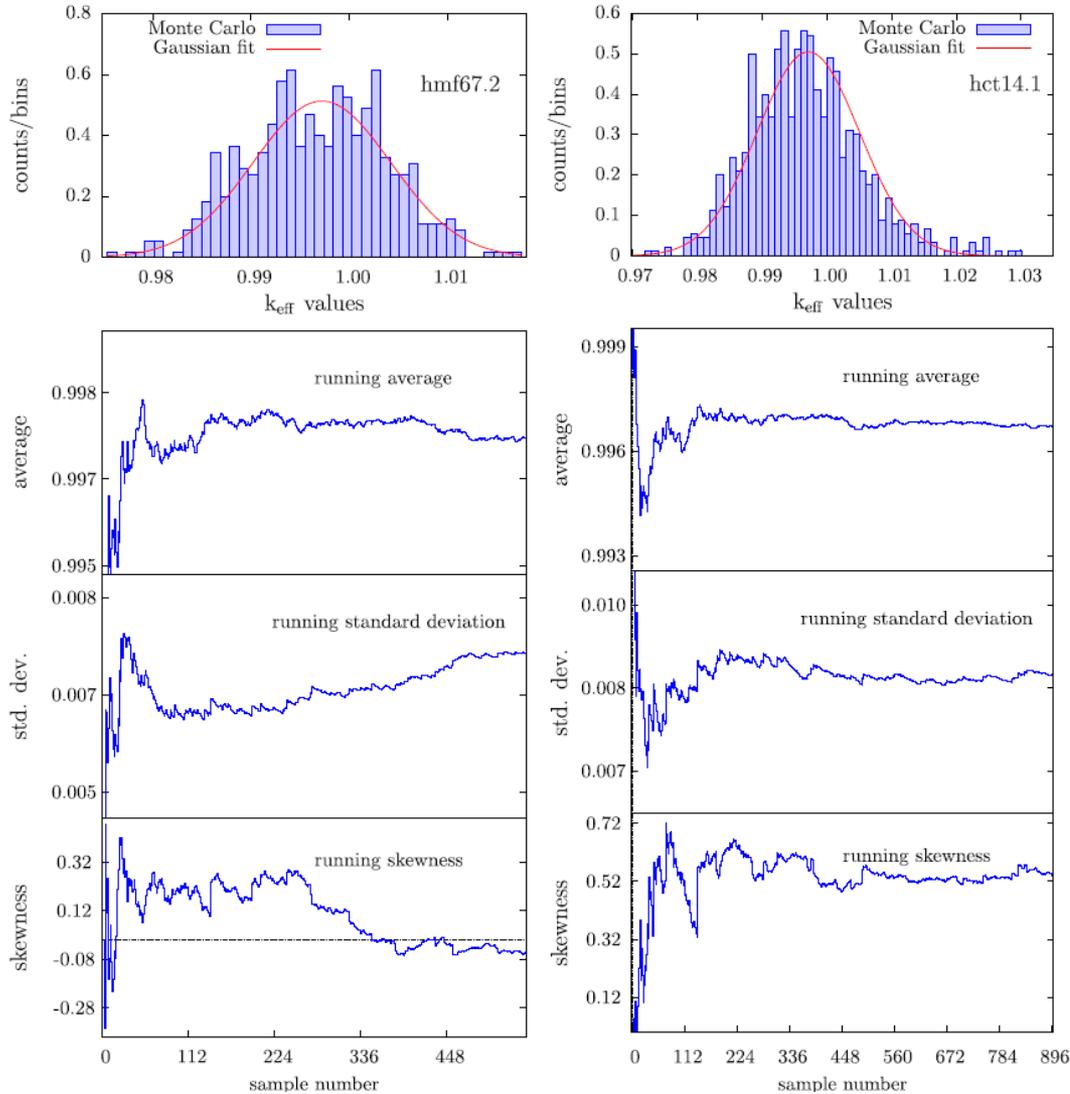
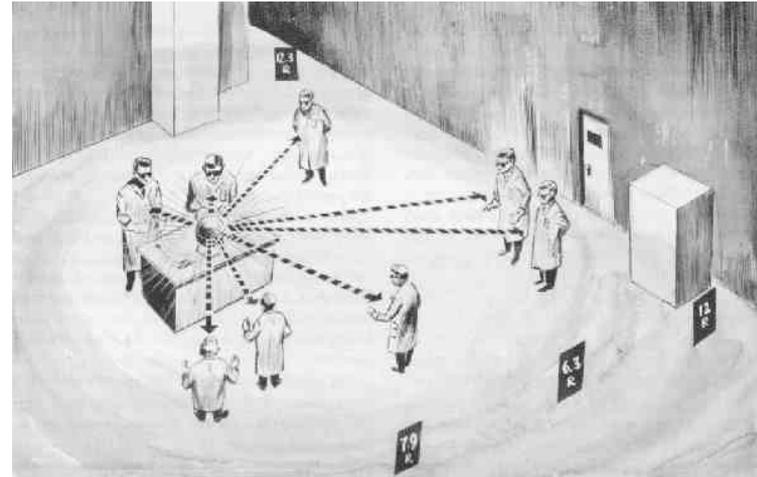


FIG. 46. (Color online) Examples of two different skewness for the same quantity, the number density of the pseudo fission product, changing the $^{238}\text{U}(n,\gamma)$ cross section at 10 keV in one case (red) and the ^{235}U fission yields in the other case (blue).

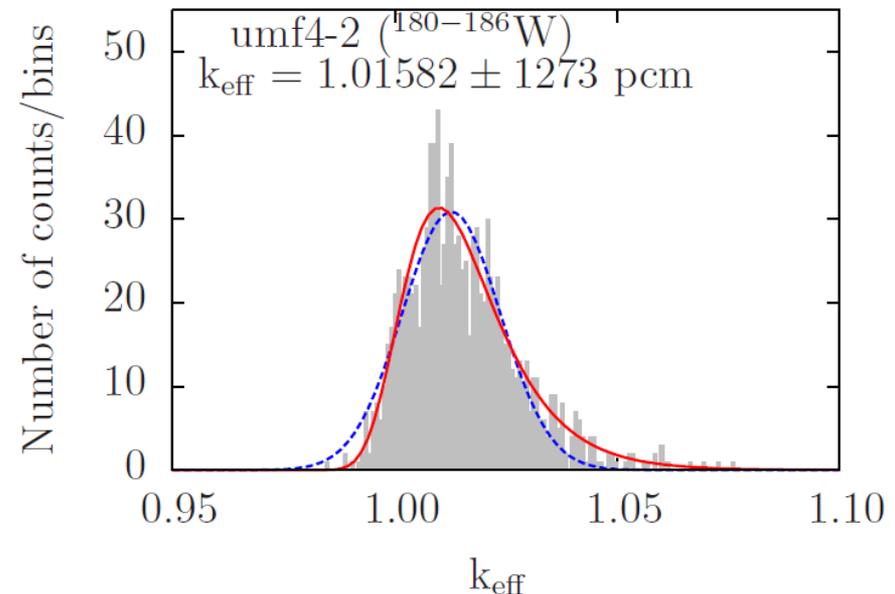
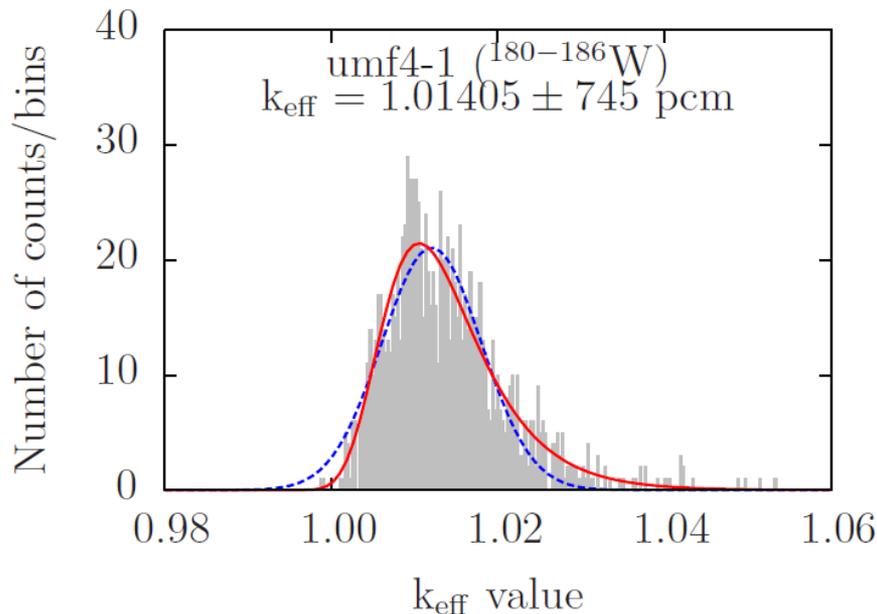
- In Monte Carlo method, the convergence of the results is a key quantity



- Criticality-safety benchmarks are crucial to assess the criticality safety of nuclear installation (fuel storage, liquid waste, fissile material storage...)
- It is all about k_{eff} and must be < 1
- Safety authorities often impose an administrative limit of 0.95 (**conservative** approach)
- Economics pushes for a “**best estimate + uncertainties**” approach
- As a consequence, 0.95 might not be valid anymore,
- As a consequence, more fissile material can be stored,
- All depending on precise estimation of the uncertainties on k_{eff} .



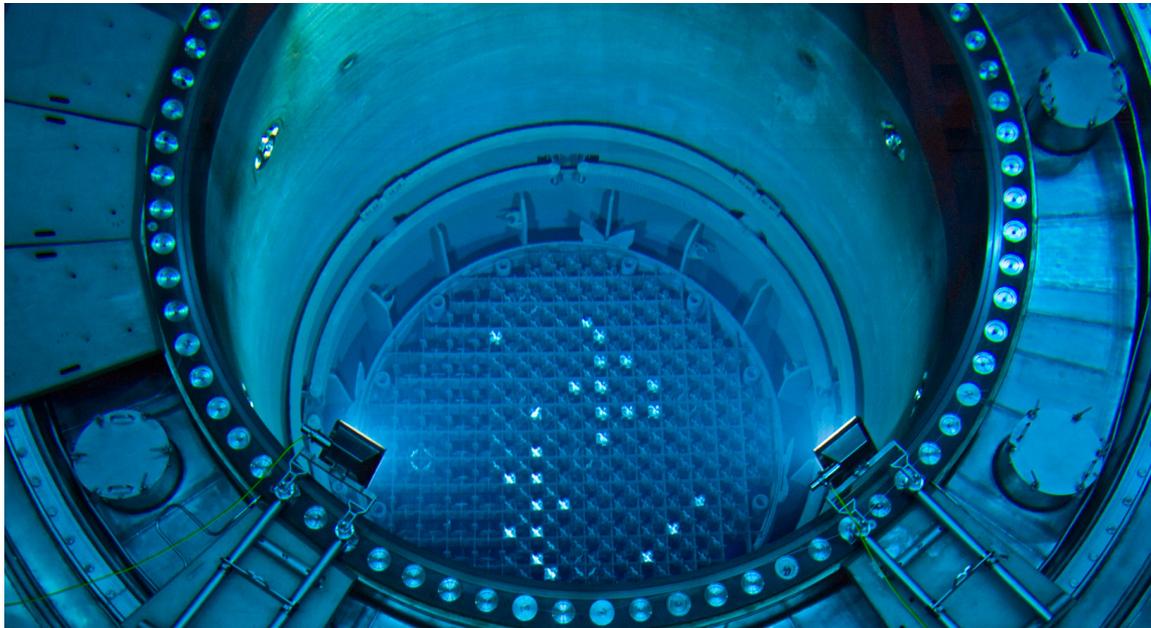
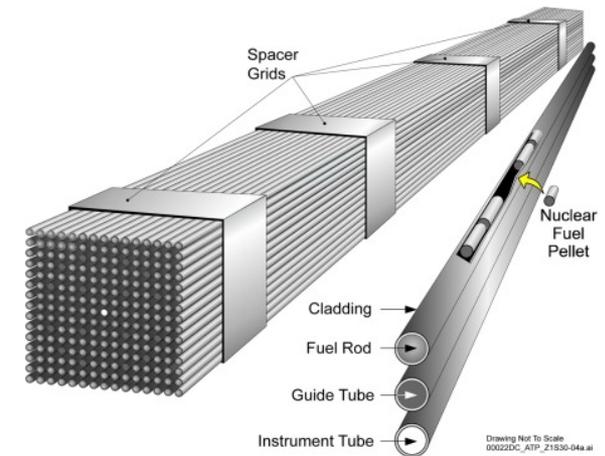
- Criticality benchmarks are used to validate codes (such as MCNP) to make sure that the calculated k_{eff} is correct.
- Additionally, Monte Carlo Uncertainty propagation method lead to “pdf”, more suitable for uncertainty-safety assessments



- The strength of the MC methods is in the access to the moments of the distributions, not reflected by a single number such as the standard deviation.

All starts with a pincell:

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



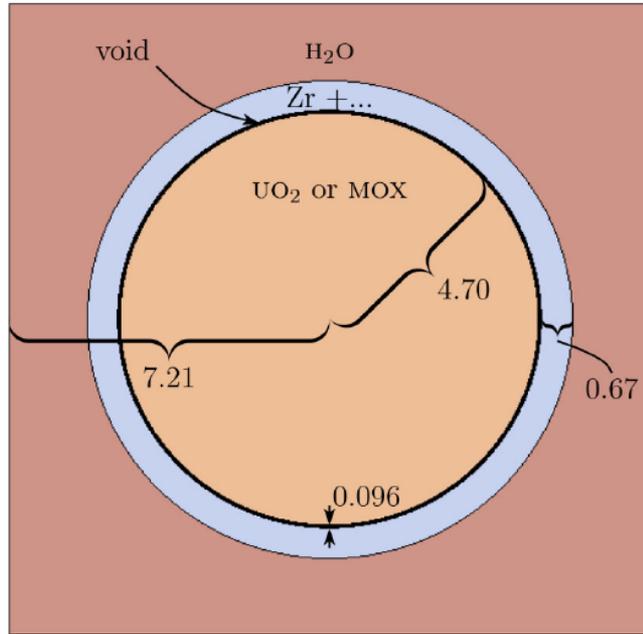


Fig. 1. The geometry of the pin cell model used in Serpent. The fuel, either UO_2 or MOX, is surrounded by concentric annular rings with a void and Zircaloy clad. The rest of the square is filled with water, and all sides are subject to reflecting boundary conditions. All distances are in millimeters.

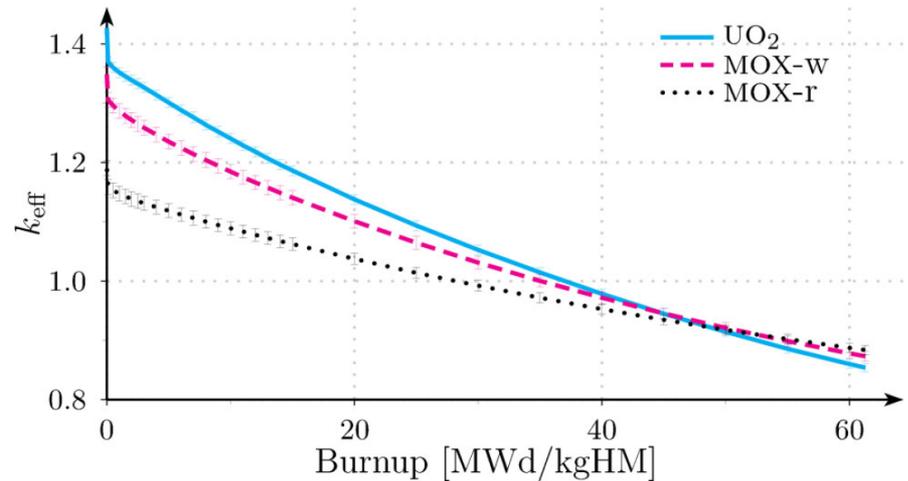


Fig. 3. $k_{\text{eff}} = k_{\infty}$ as a function of burnup for the three fuel types. The large deviations from 1 are explained by the simplified model: no leakage, infinite grid of pin cells (with the same burnup), and no control mechanisms. The uncertainty bars represent the data uncertainty $\sigma_{\text{data}}(k_{\text{eff}})$;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

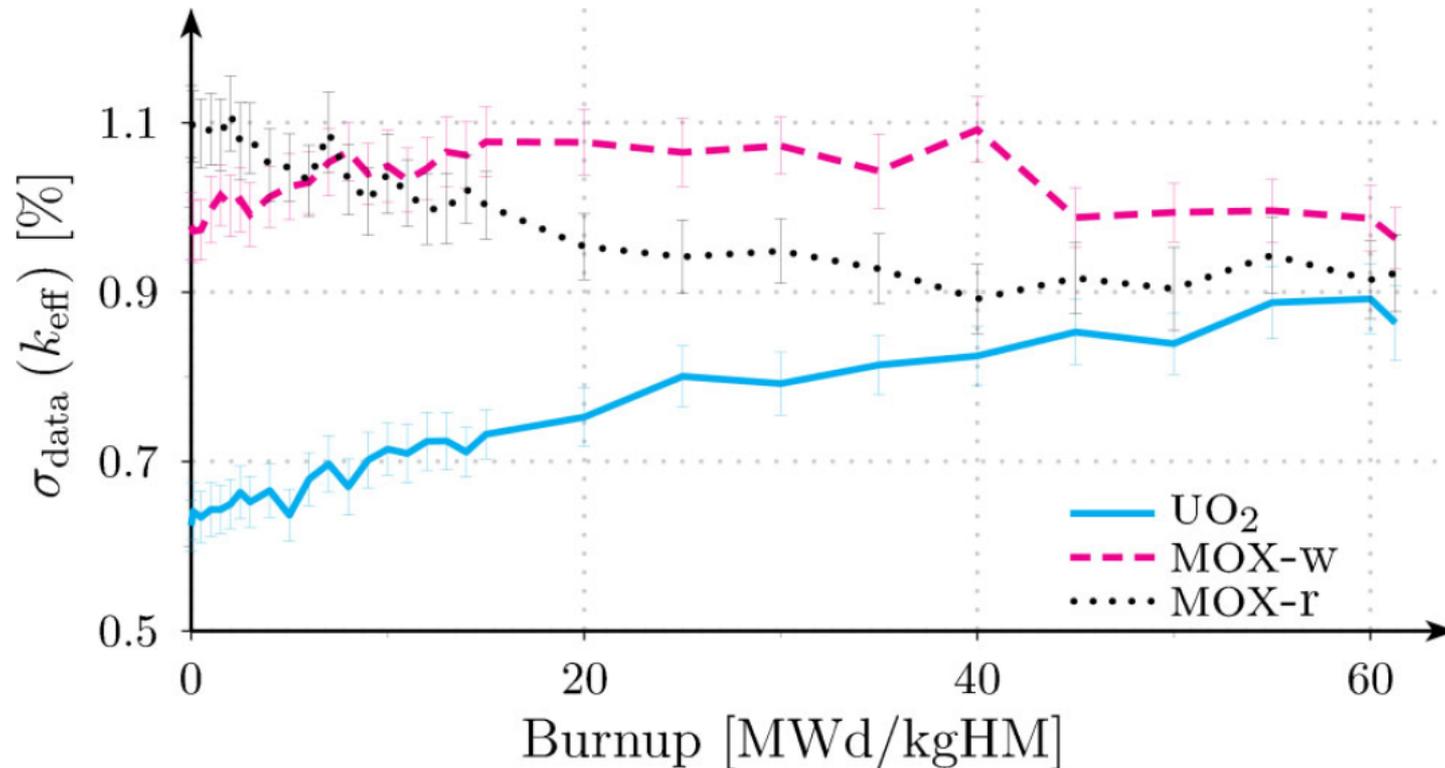


Fig. 2. The main result: Propagated data uncertainty in k_{eff} for UO₂ and the two types of MOX fuel as functions of burnup due to all data. The uncertainty bars represent one standard deviation.

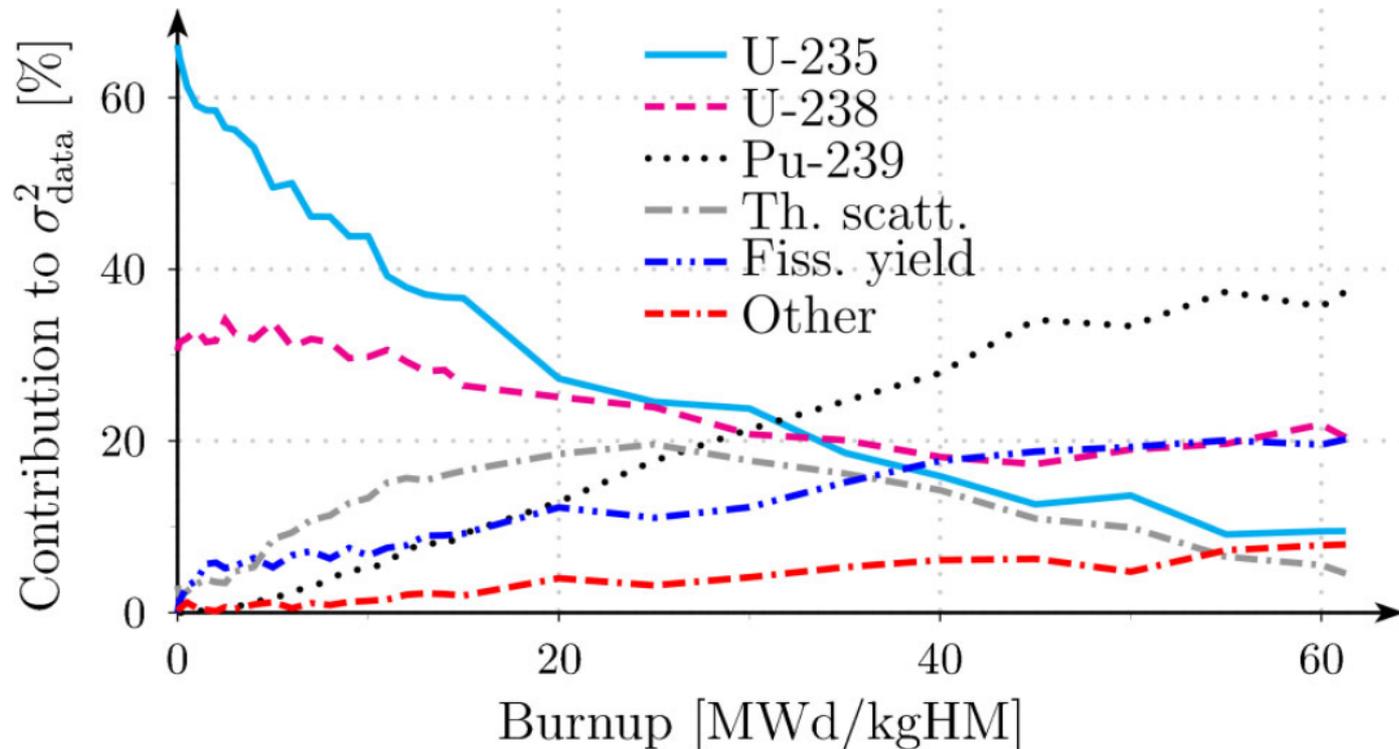
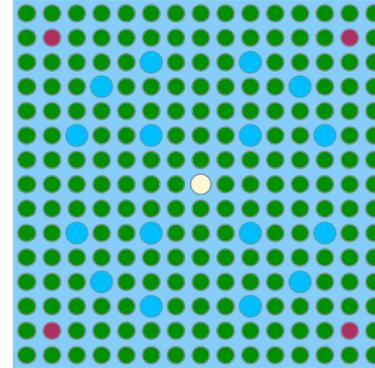


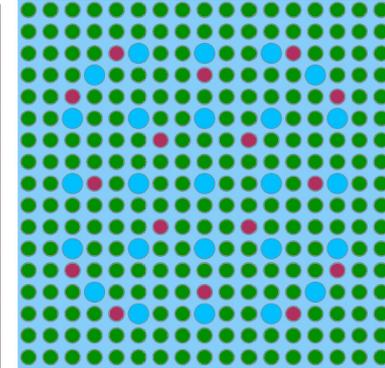
Fig. 4. Contributions to total variance in k_{eff} from variance of individually varied data, for UO_2 . “Other” stands for transport and activation data of fission products and minor actinides.

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

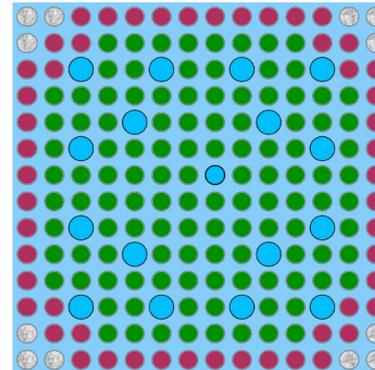
PWR UO_2



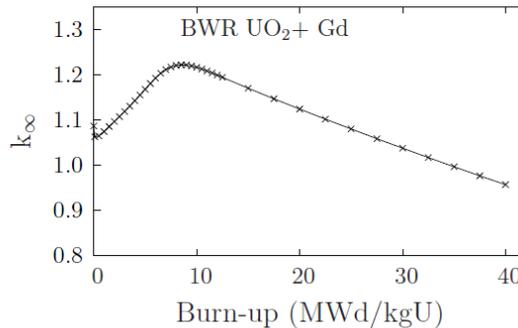
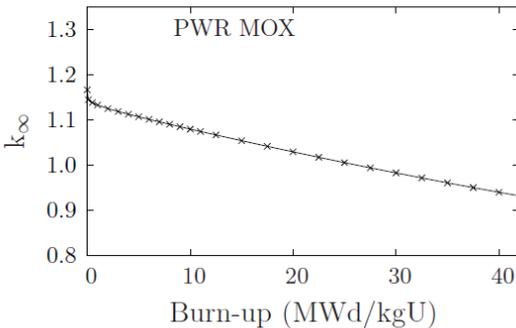
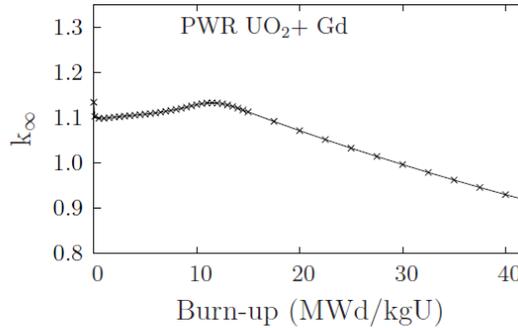
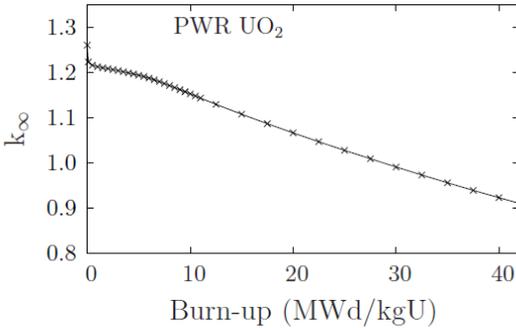
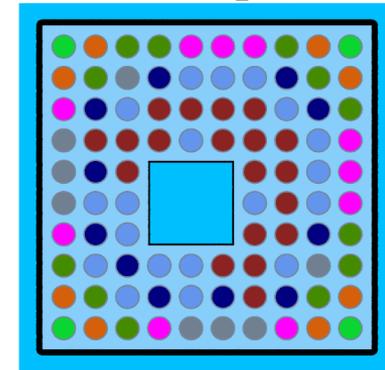
PWR $UO_2 + Gd$



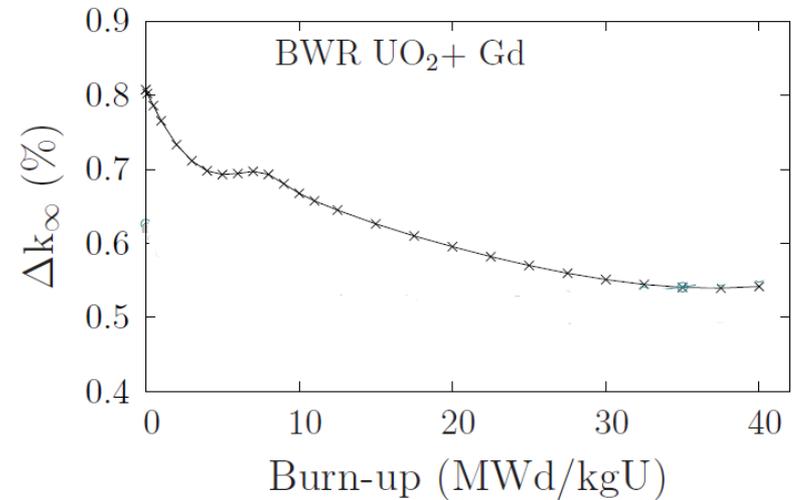
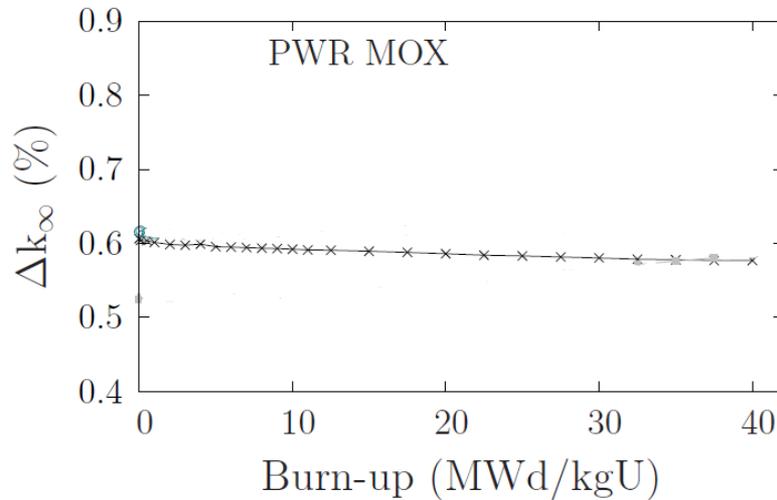
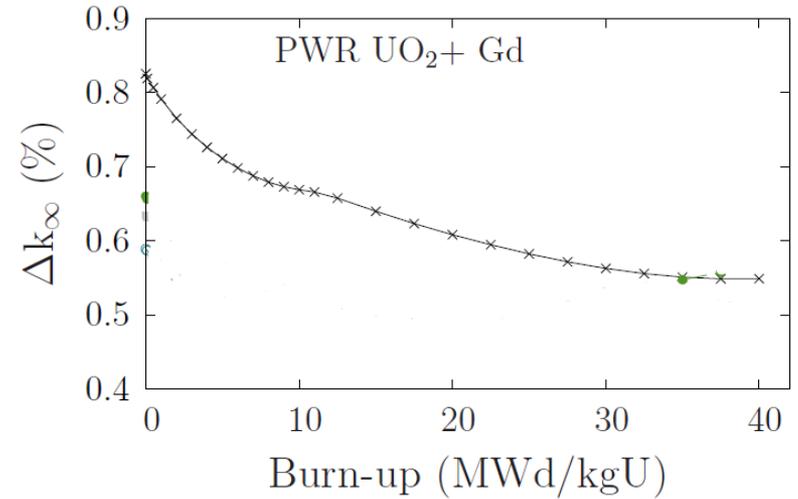
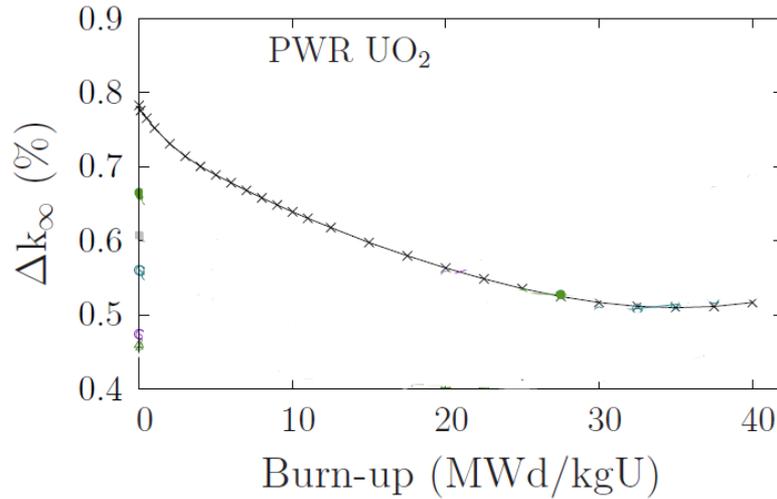
PWR MOX



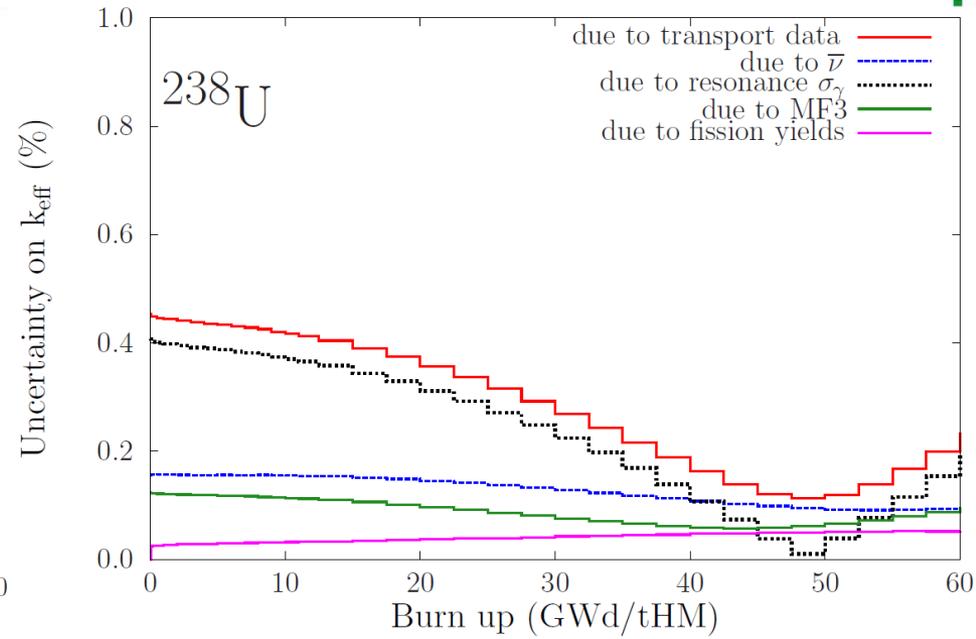
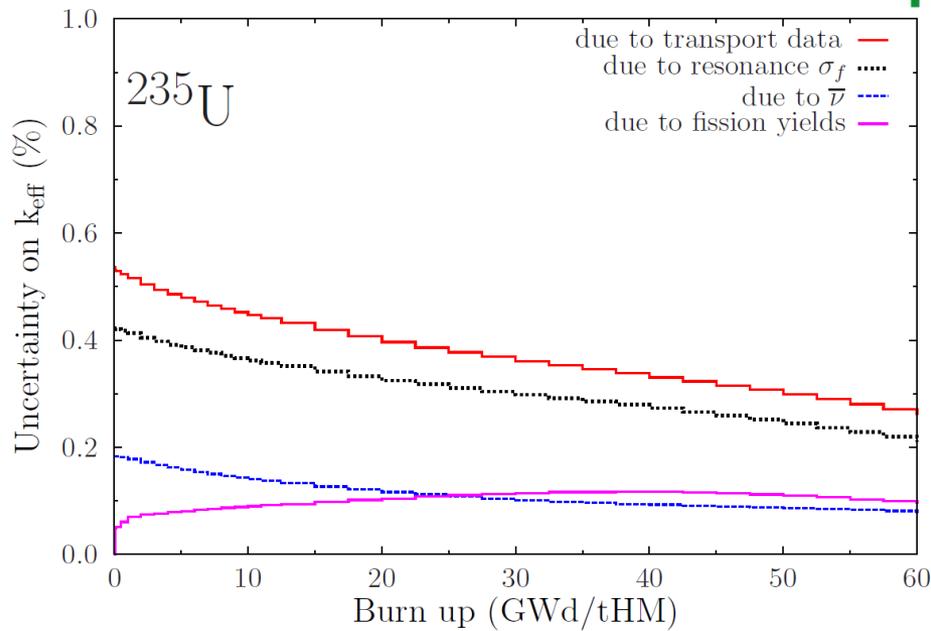
BWR $UO_2 + Gd$



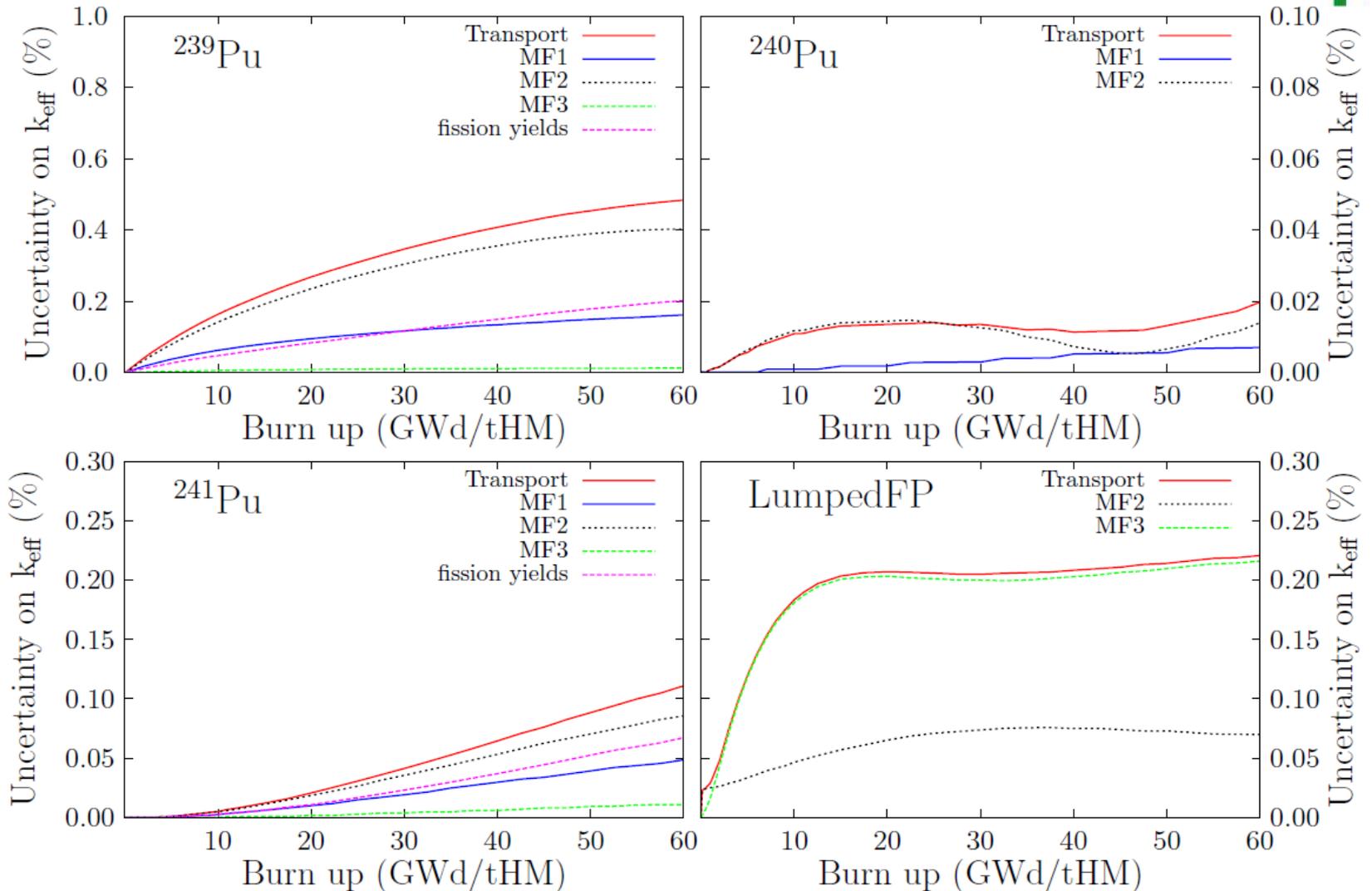
- K_{inf} uncertainty for 4 assemblies, 1 reactor cycle



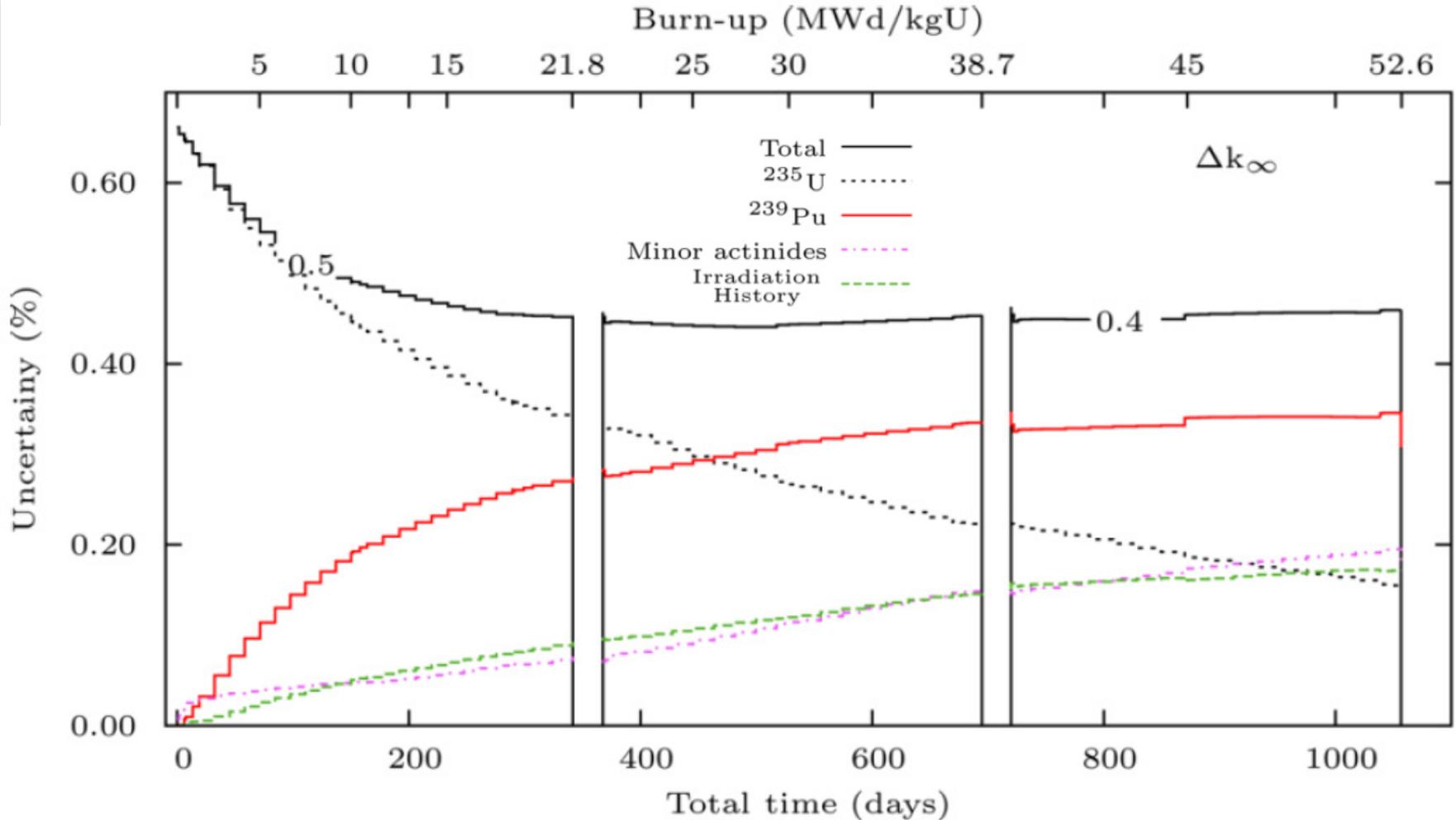
- K_{inf} uncertainty contributions

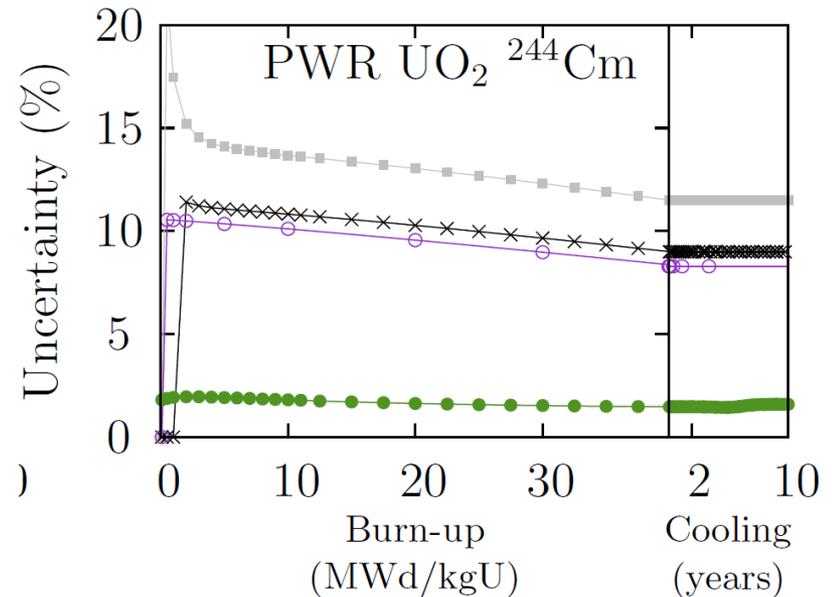
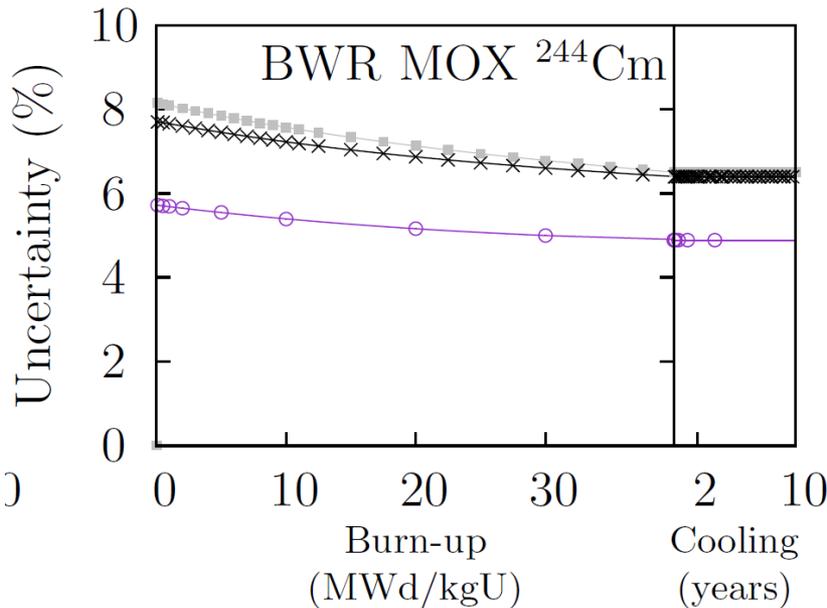
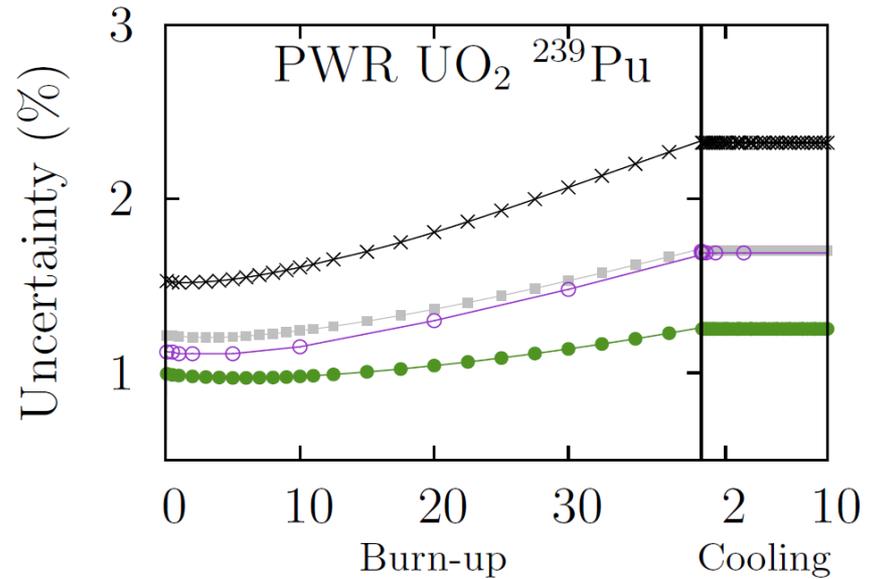
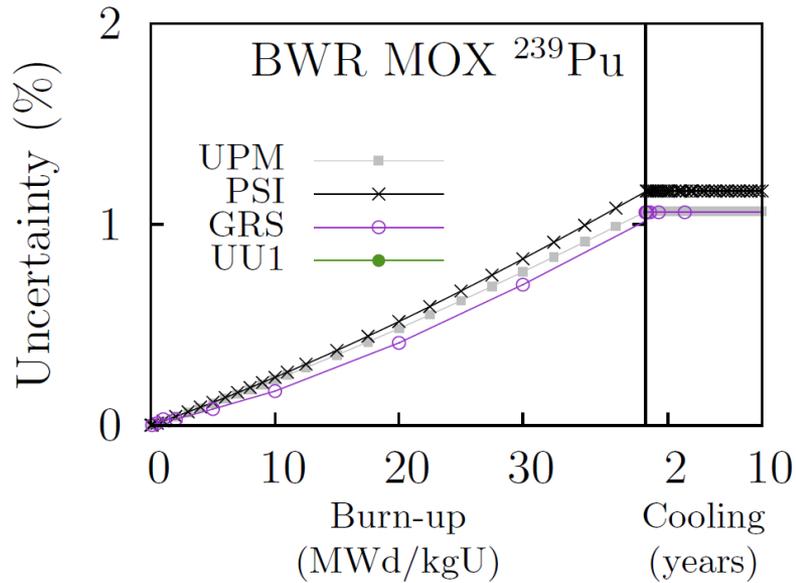


- K_{inf} uncertainty contributions



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





- Uncertainty at different locations due to nuclear data,
- For different quantities (inventory, boron concentration, power distribution, safety parameters such as Linear Heat Generation rate...)
- No sensitivity method can be applied

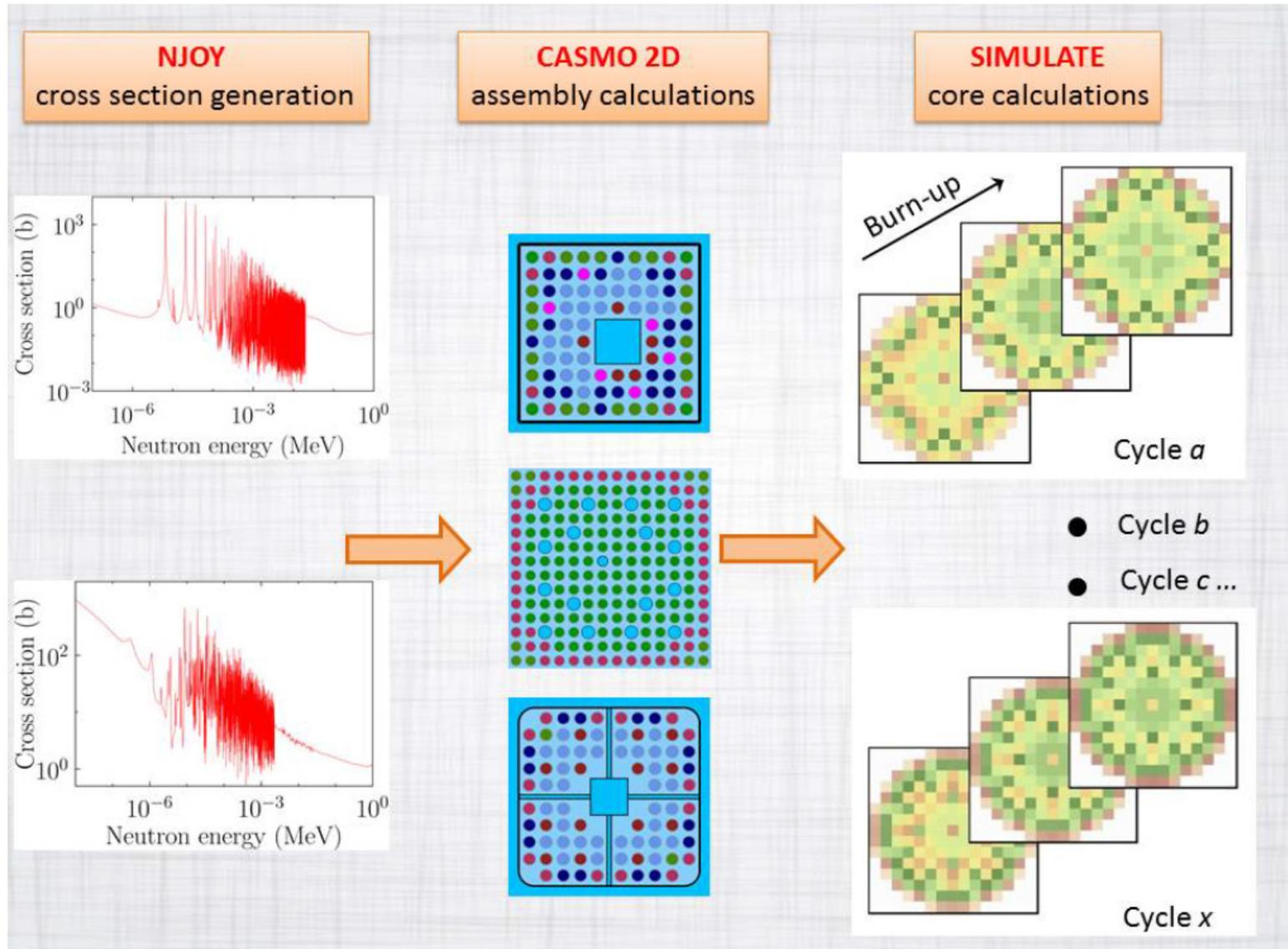
CYCLE MOX

	1	2	3	4	5	6	7	8	9	10	11	12	13
A						29	34	30					
B				30	0	0*	10	0*	0	27			
C			30	0	8*	32	6	32	8*	0	30		
D		27	0	15	19	9	30	9	19	15	0	30	
E		0	8*	19	17*	29	10*	28	17*	19	8*	0	
F	30	0*	32	9	28	10	17	10	29	9	32	0*	29
G	34	10	6	30	10*	17	27*	17	10*	30	6	10	34
H	29	0*	32	9	29	10	17	10	28	9	32	0*	30
I		0	8*	19	17*	28	10*	29	17*	19	8*	0	
J		30	0	15	19	9	30	9	19	15	0	27	
K			30	0	8*	32	6	32	8*	0	30		
L				27	0	0*	10	0*	0	30			
M						30	34	29					

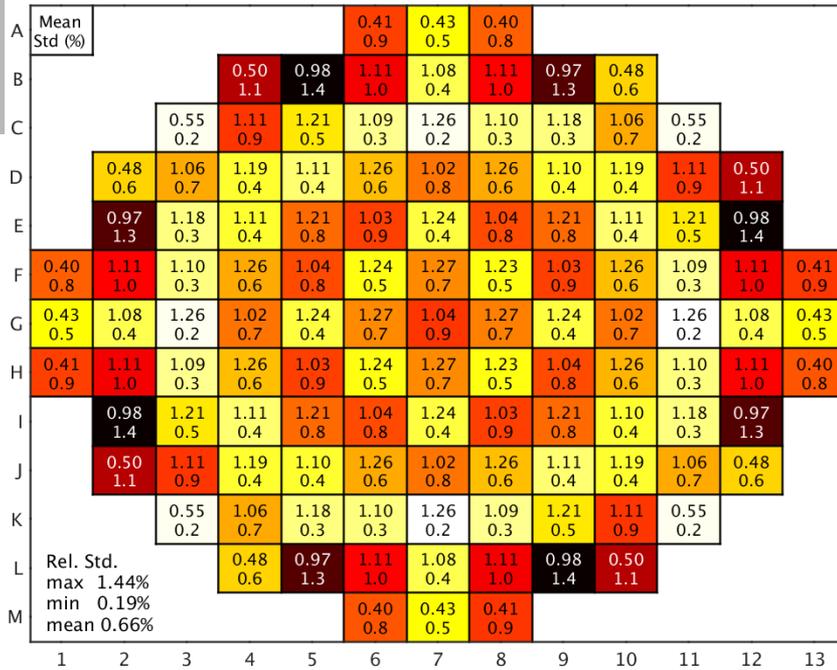
CYCLE UOX

	1	2	3	4	5	6	7	8	9	10	11	12	13
A						57	55	57					
B				47	38	0*	0	0*	37	47			
C			55	0	11*	47	51	47	11*	0	55		
D		47	0	37	36	11	38	11	36	37	0	47	
E		37	11*	36	25*	24	25*	24	25*	36	11*	38	
F	57	0*	47	11	24	25	39	25	24	11	47	0*	57
G	55	0	51	38	25*	39	53*	39	25*	38	51	0	55
H	57	0*	47	11	24	25	39	25	24	11	47	0*	57
I		38	11*	36	25*	24	25*	24	25*	36	11*	37	
J		47	0	37	36	11	38	11	36	37	0	47	
K			55	0	11*	47	51	47	11*	0	55		
L				47	37	0*	0	0*	38	47			
M						57	55	57					

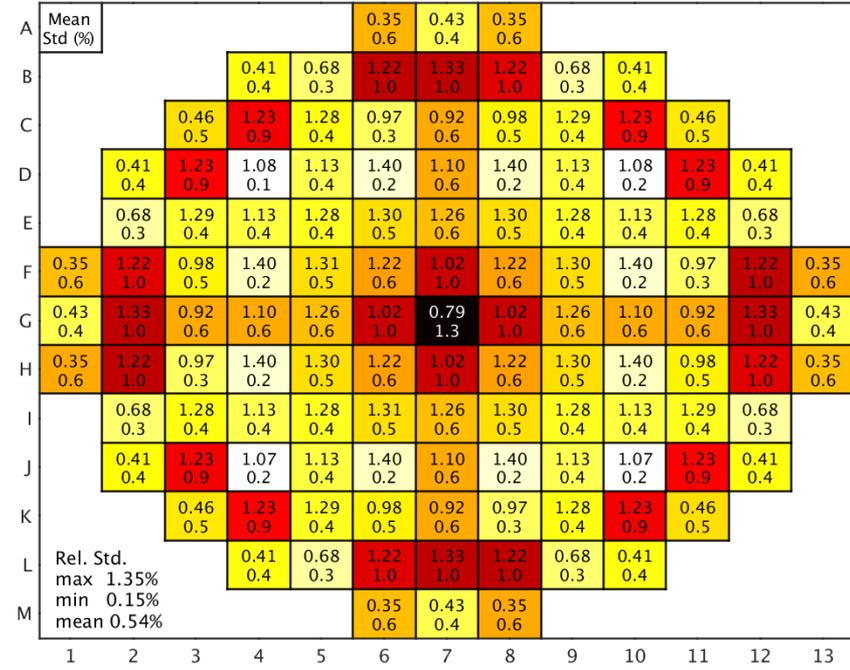
- Example with CASMO/SIMULATE,



- Example with CASMO/SIMULATE,

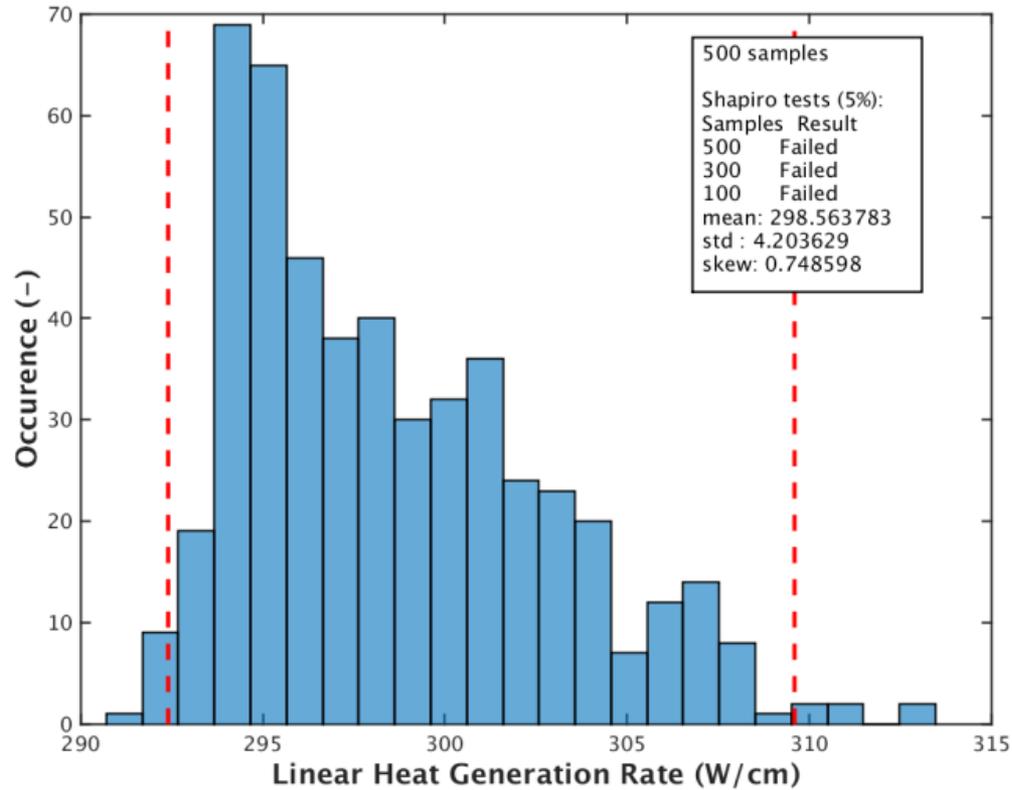


Relative radial power distributions of the MOX



Relative radial power distributions of the UO₂

- Asymmetric distributions for safety parameters



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

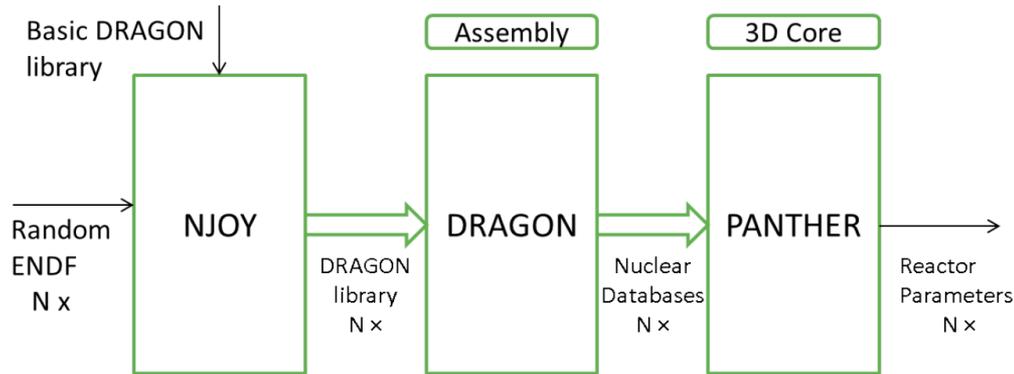


Figure 1. Calculation scheme for the determination of the uncertainties in the main reactor parameters due to nuclear data uncertainties.

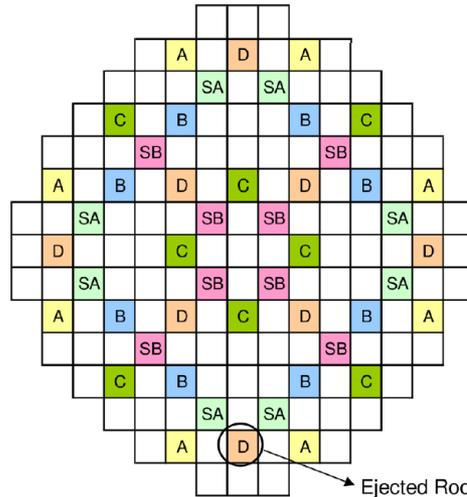
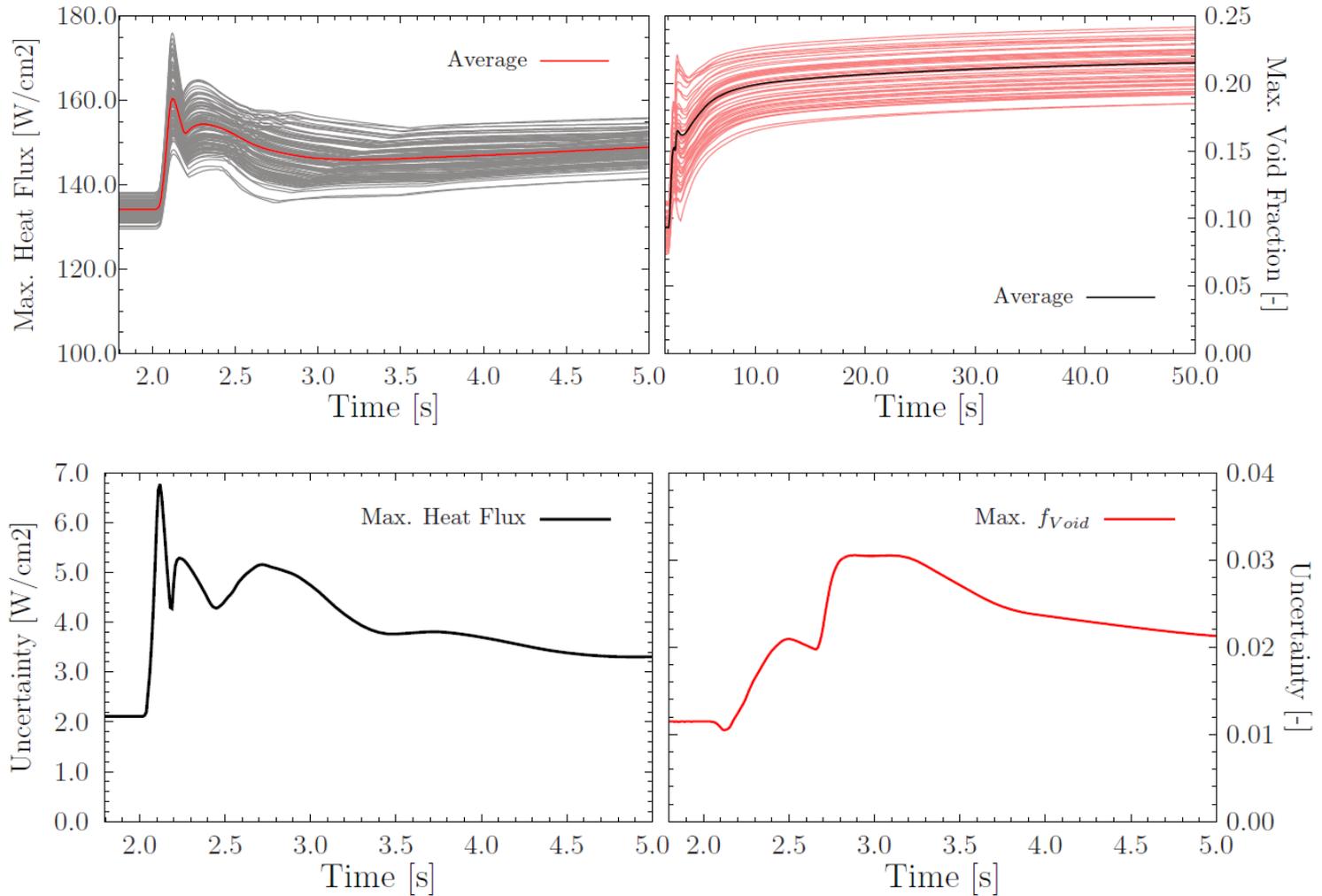
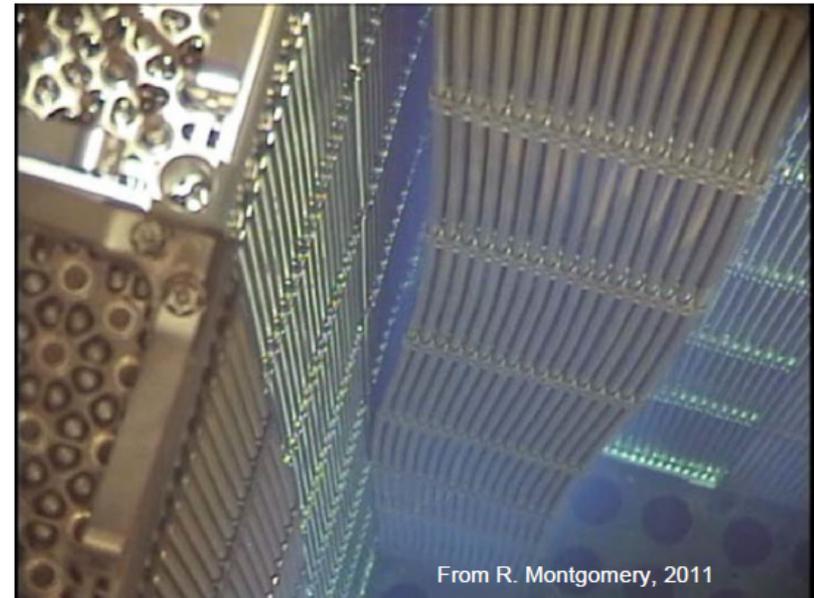
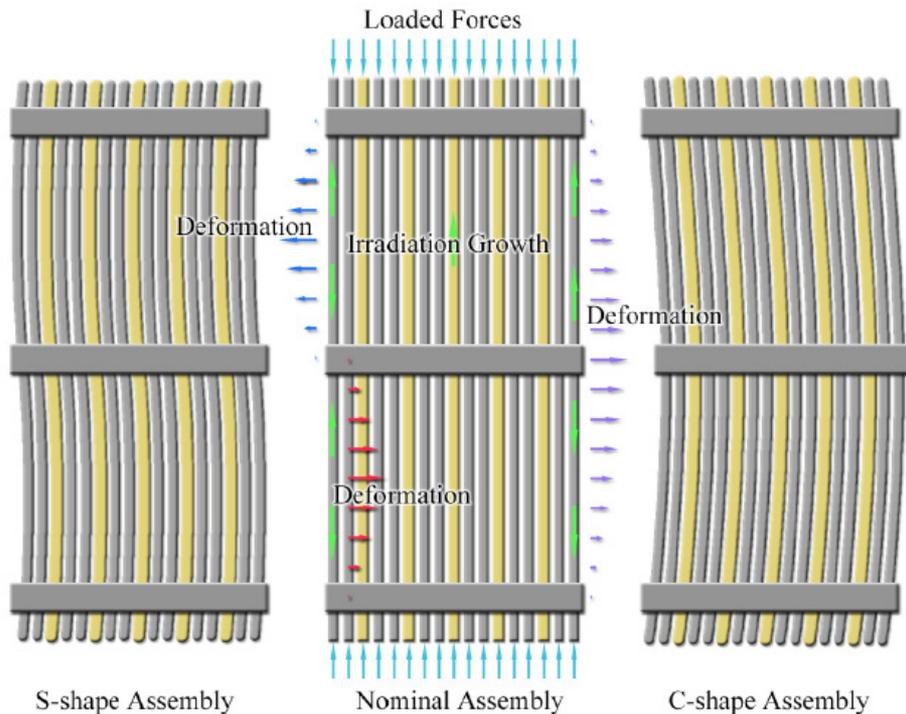


Figure 2. Scheme of Westinghouse core with distribution of control rod banks and position of the ejected control rod.

- Control Rod Ejection Accident, with ND uncertainties

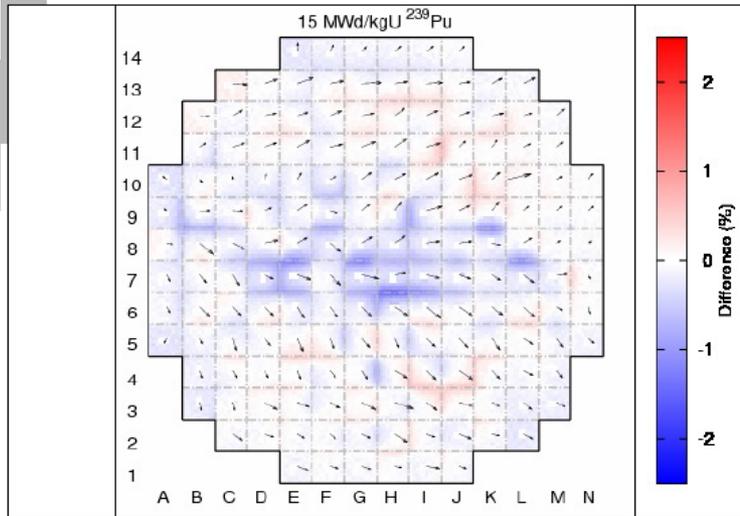


- Bowing effect: deformation of the fuel assemblies observed in PWR and BWR,
- Impact on the motion of control rods,
- Impact on isotopic content, power map...
- And impact on the safe operation of the reactor

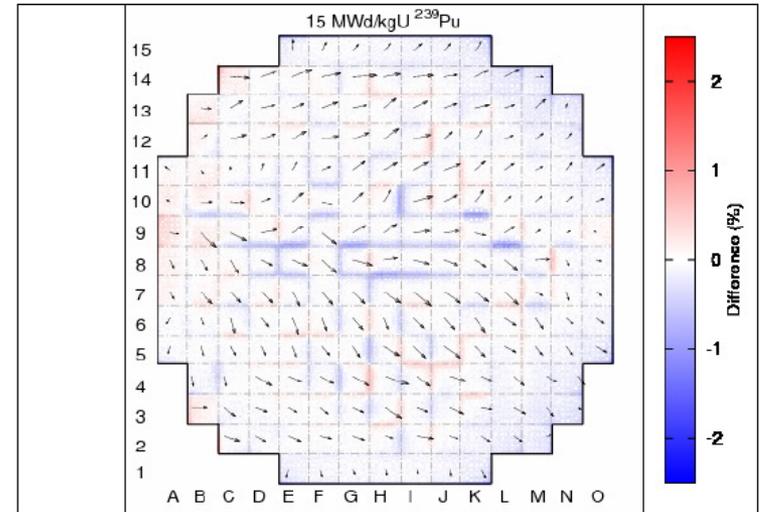


6. Example for the bowing effect

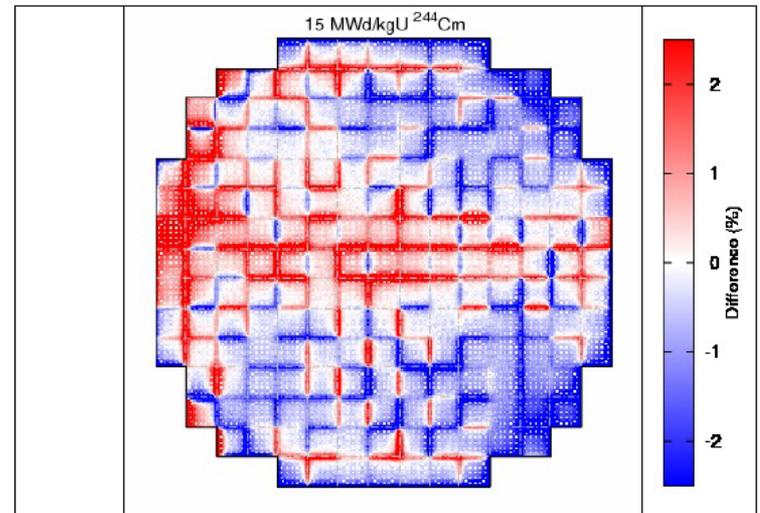
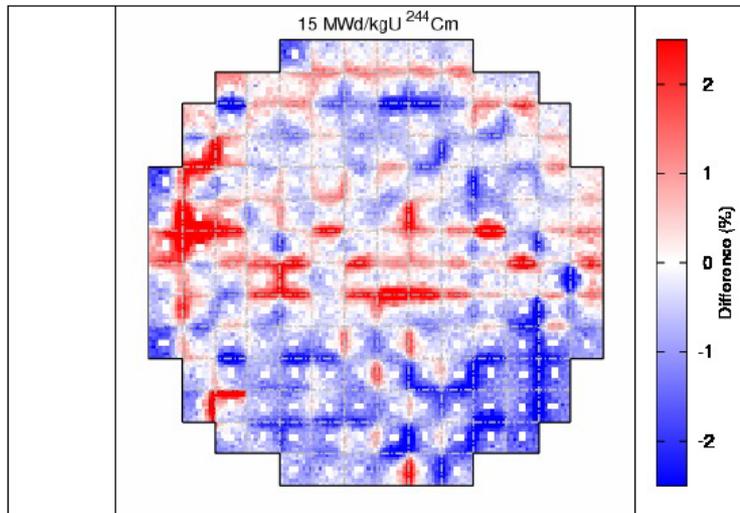
- isotopic content for ^{239}Pu and ^{244}Cm (to be compared with the nuclear data effect)



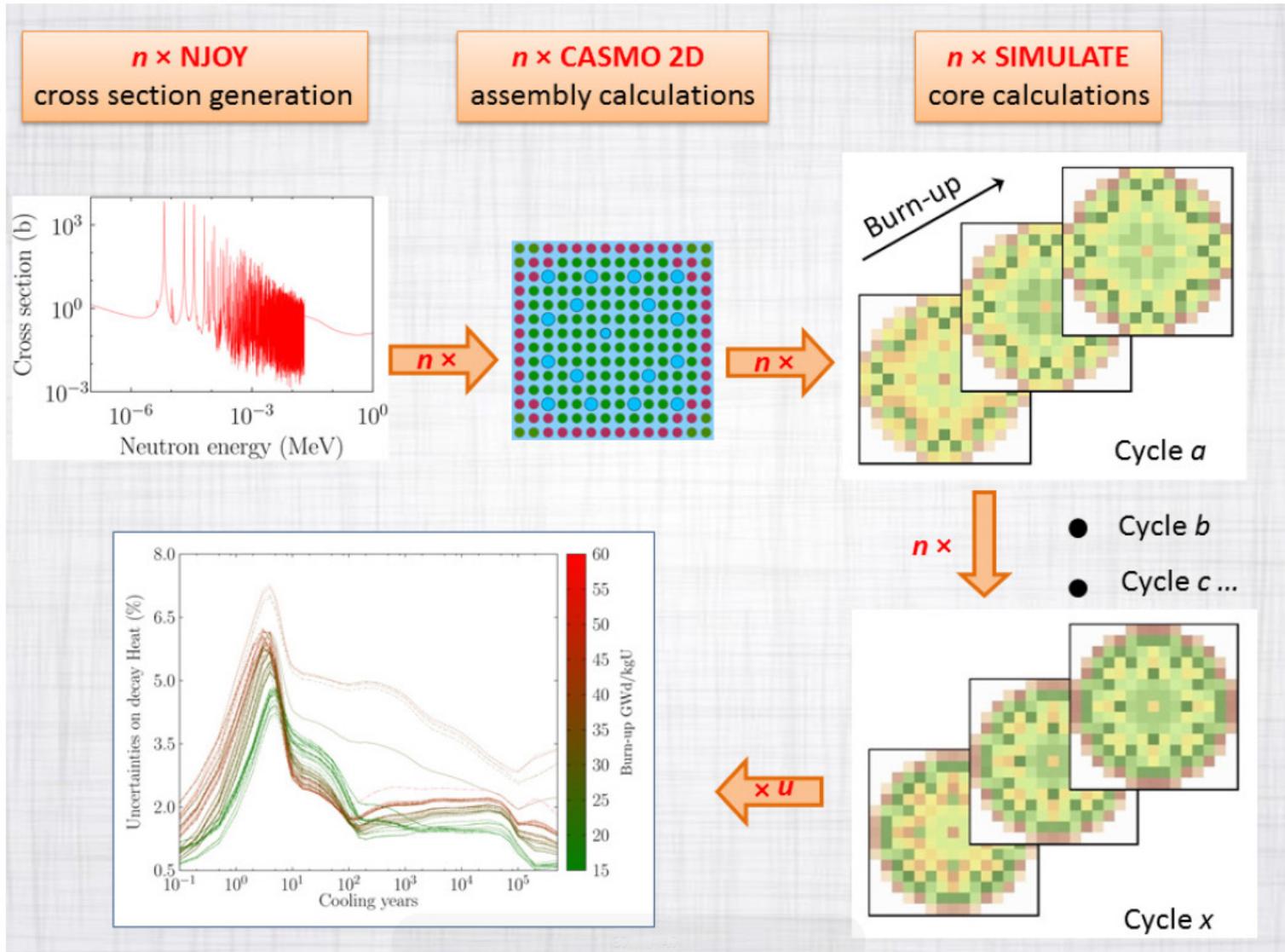
BWR



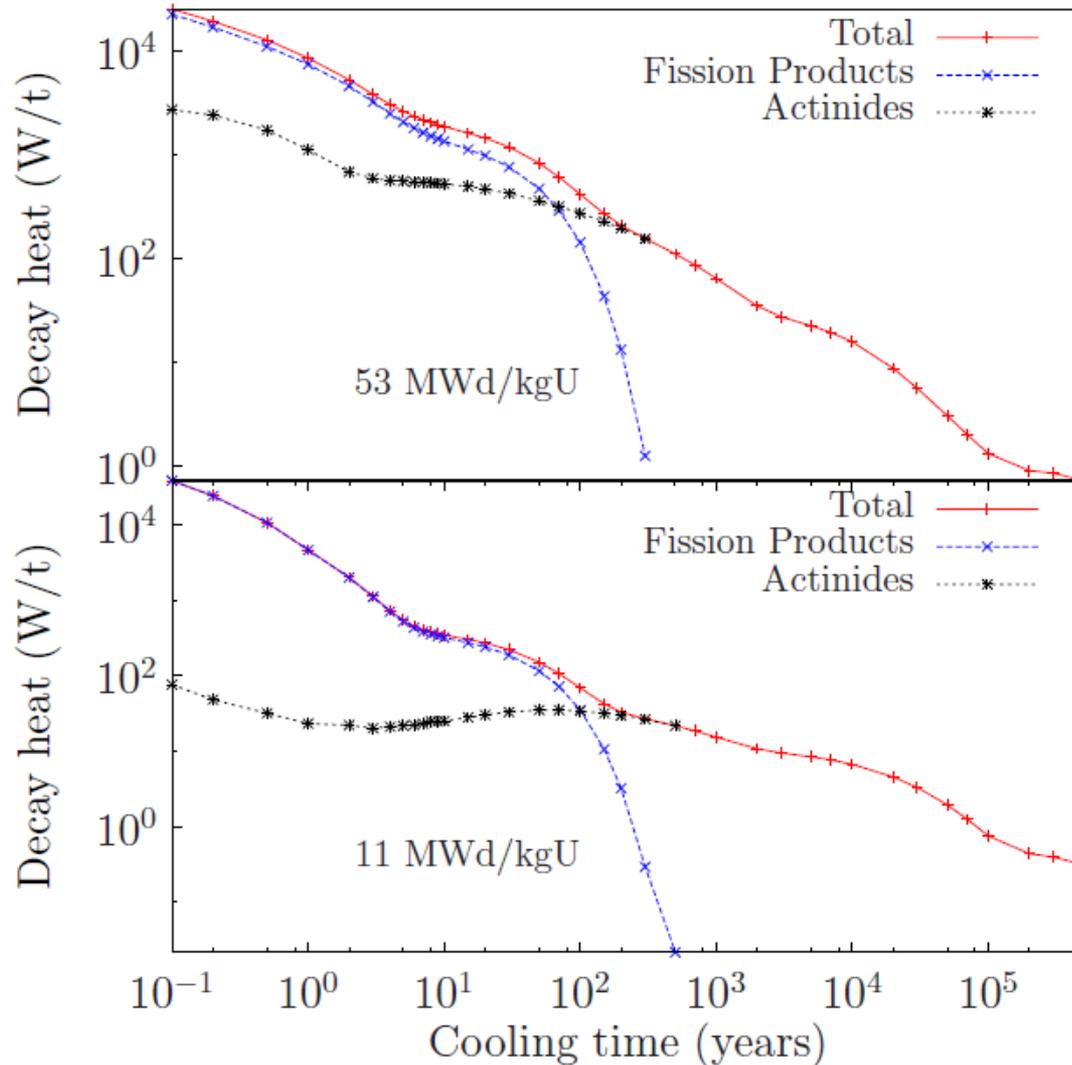
PWR



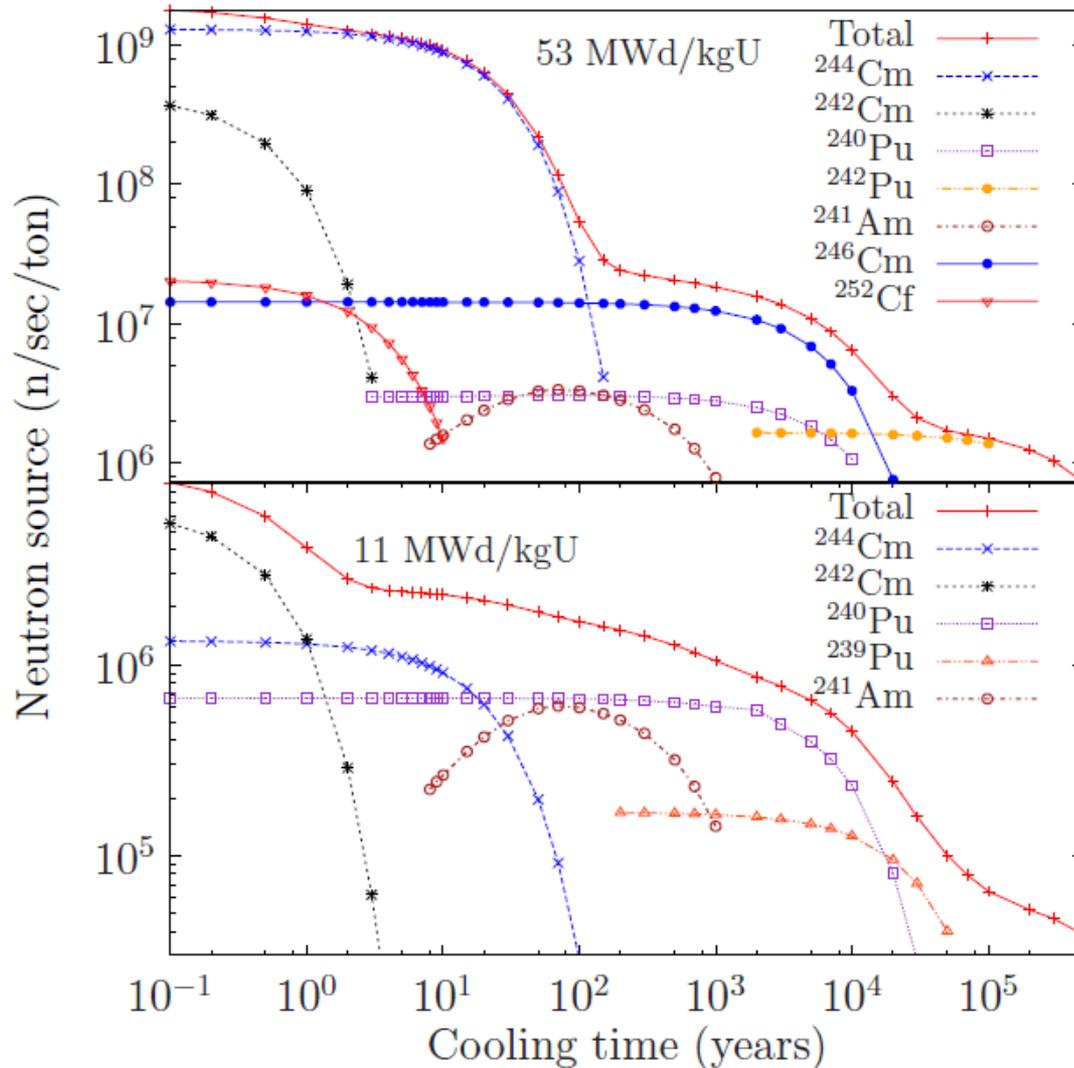
- Total Monte Carlo approach: random nuclear data for the full calculation chain.



- Important quantities: decay heat, isotope inventory, neutron/gamma source and criticality

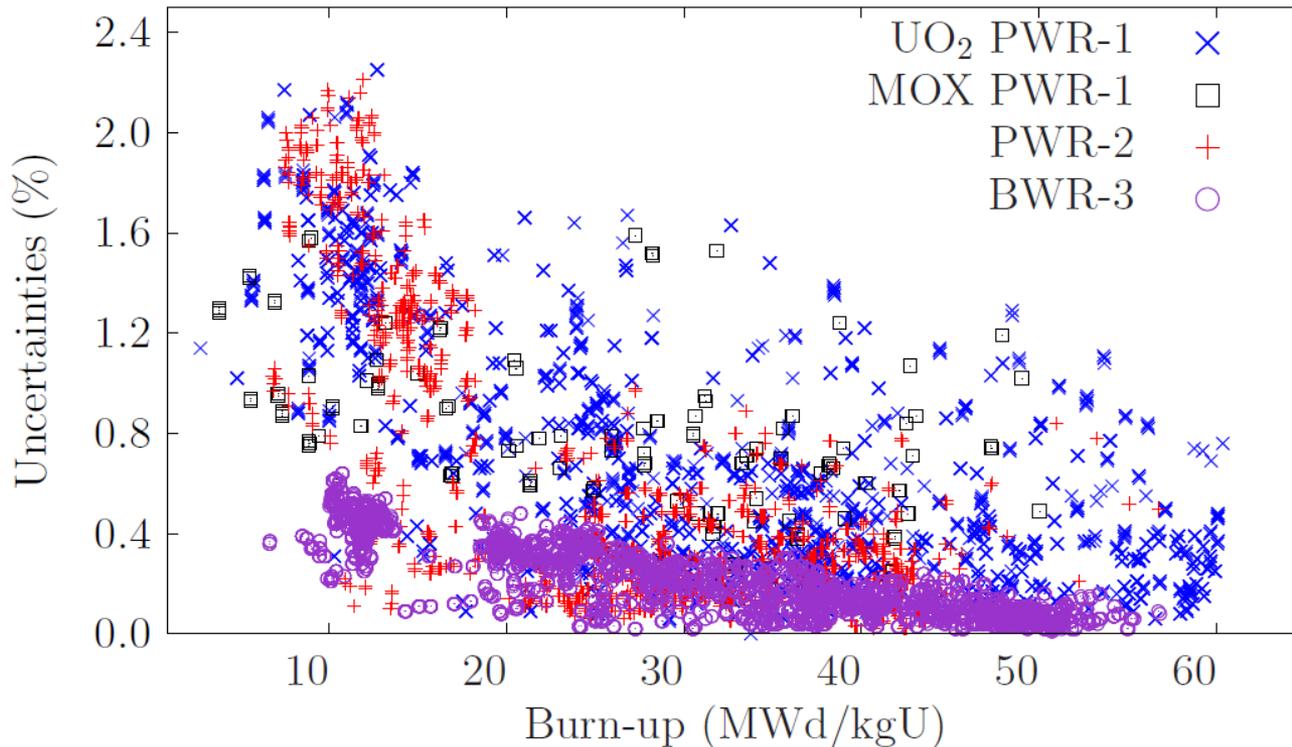


- Important quantities: decay heat, isotope inventory, neutron/gamma source and criticality

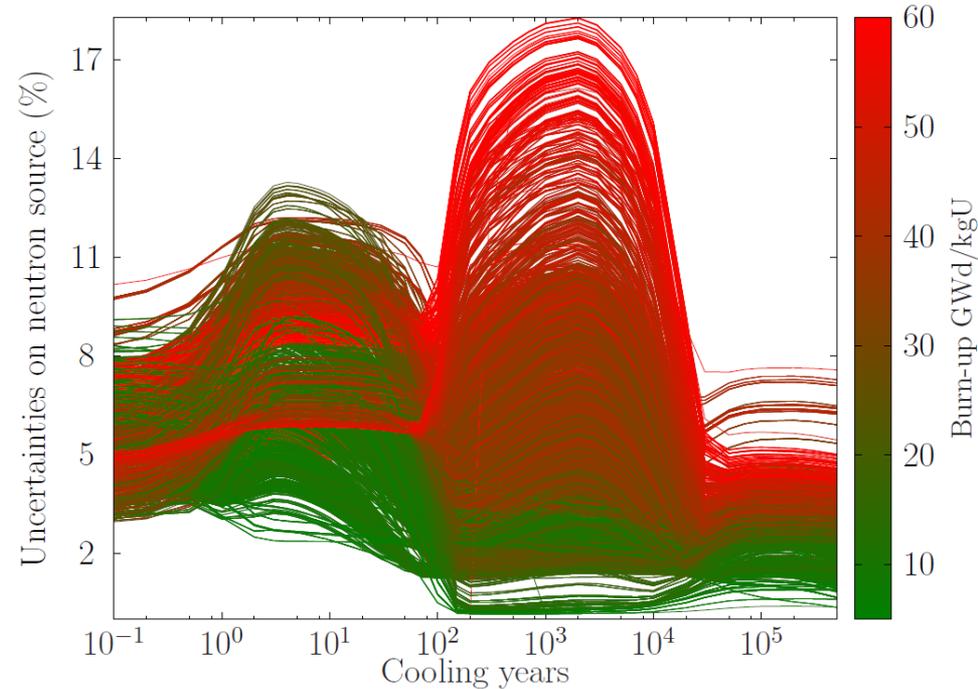
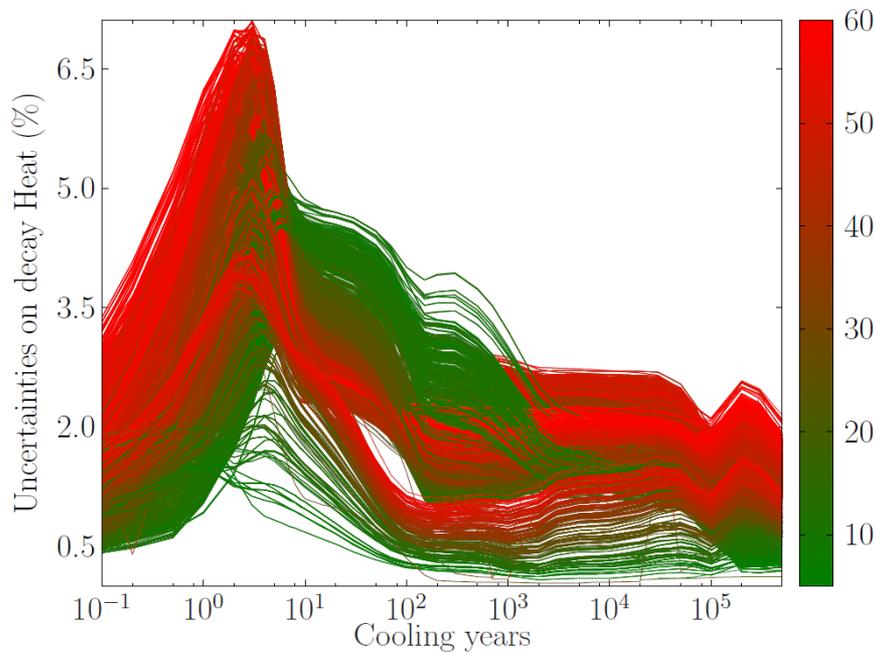


- Important quantities: decay heat, isotope inventory, neutron/gamma source and criticality

Core label	Type	Fuel	Enrichment %	Cycles	Assembly-cycles	Burn-up MWd/kgU	random cases FY	cases <i>n</i> other
PWR-1	PWR	UO ₂	2.9-4.7	17-42	2542	4-60	320	110
PWR-1	PWR	MOX	2.2-5.8	17-42	297	4-50	320	110
PWR-2	PWR	UO ₂	1.9-3.5	1-16	2647	7-55	110	100
BWR-1	BWR	UO ₂	0.7-4.5	19-44	3746	10-45	35	35



- Important quantities: decay heat, isotope inventory, neutron/gamma source and criticality



- A loading curve tells us how many assemblies can be put together in a canister without creating a criticality incident.
- It depends on the fuel type, enrichment, burnup...
- 100 000s of spent fuel assemblies are waiting for final disposal
- Here is a Swiss example for a specific PWR:

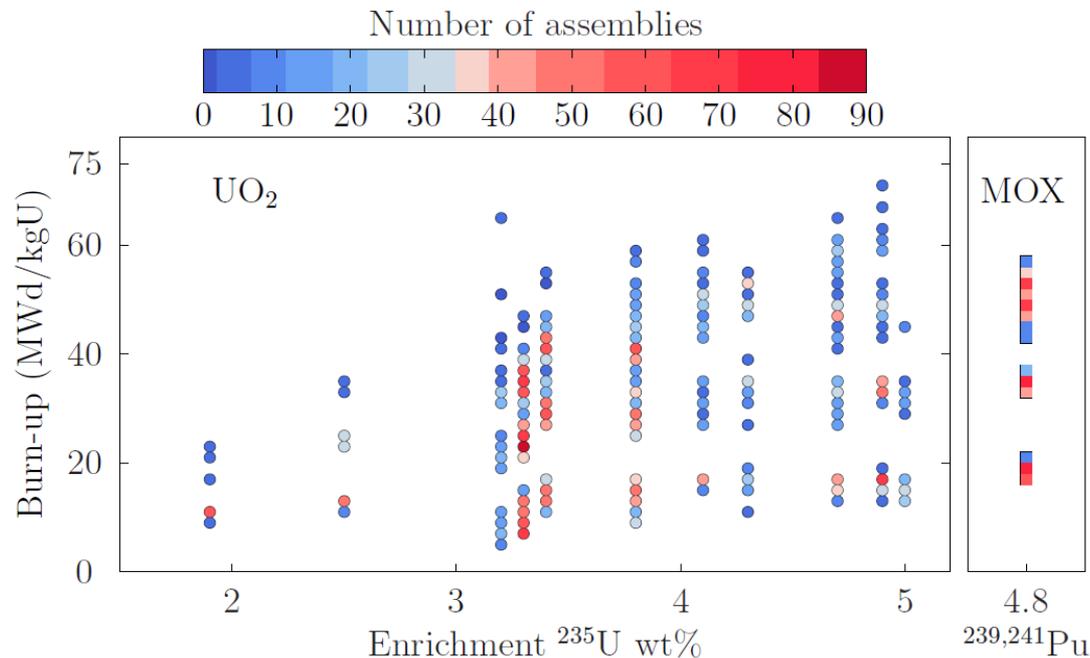
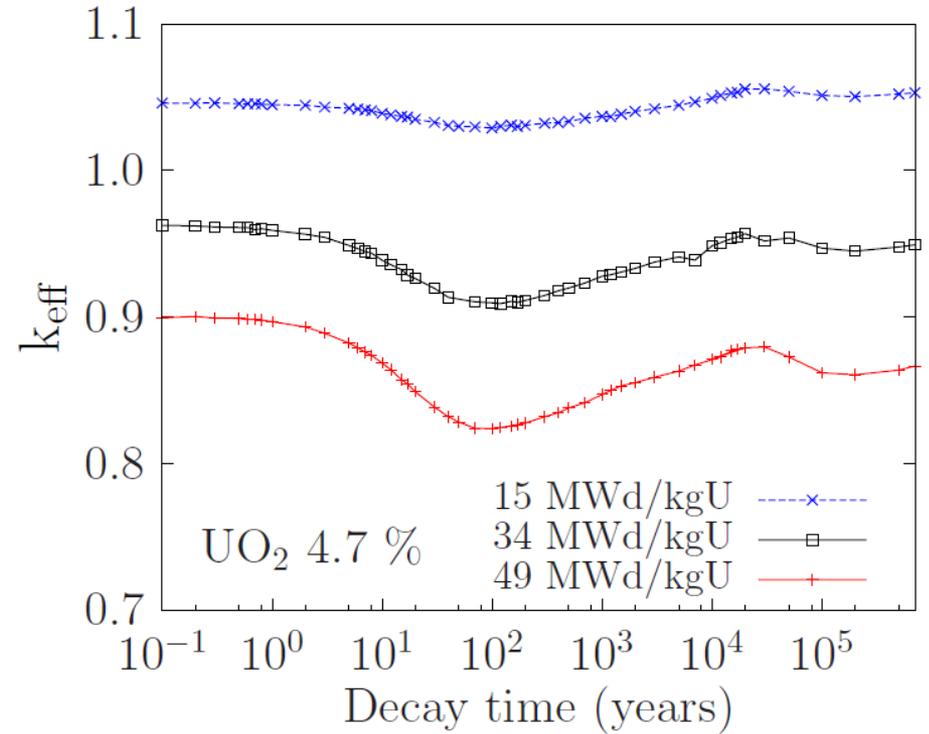
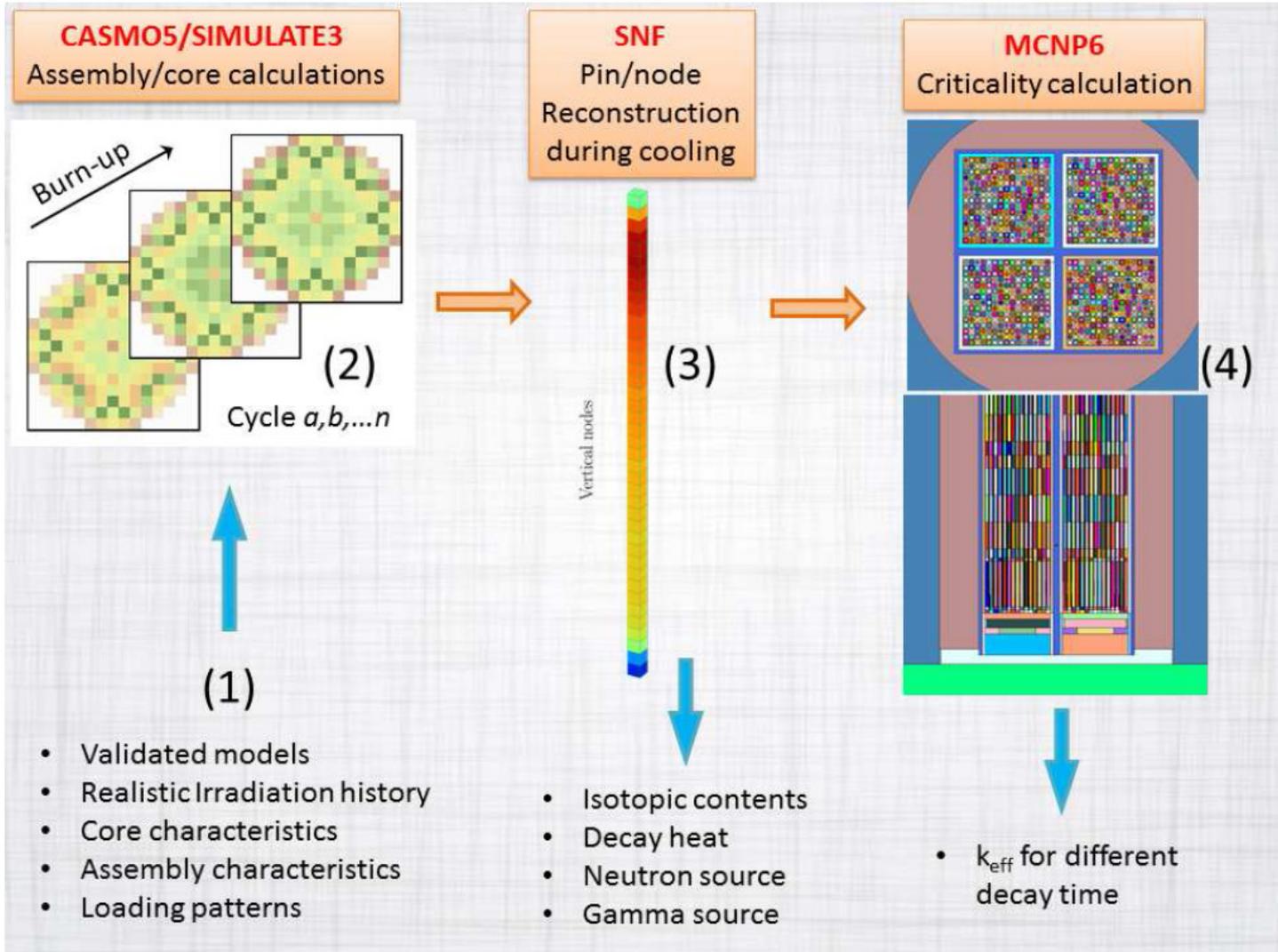


Fig. 1. Total number of fuel assemblies considered in this work from a specific Swiss PWR power plant, over 34 cycles (5378 UO₂ and 640 MOX assemblies). All assemblies are considered at the end of each cycle, being discharged or not.

- Criticality calculations, where is the limit ?



- Criticality calculations, where is the limit ?



- Criticality calculations, where is the limit ? **No uncertainties from nuclear data**

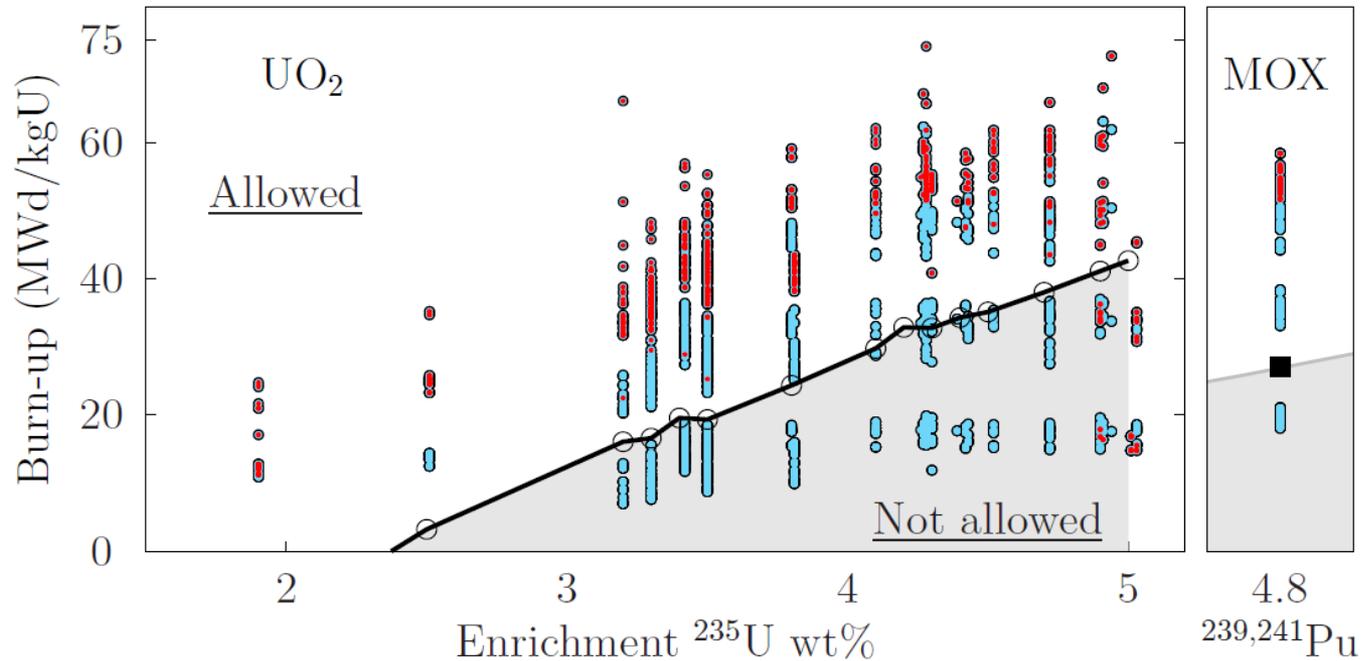
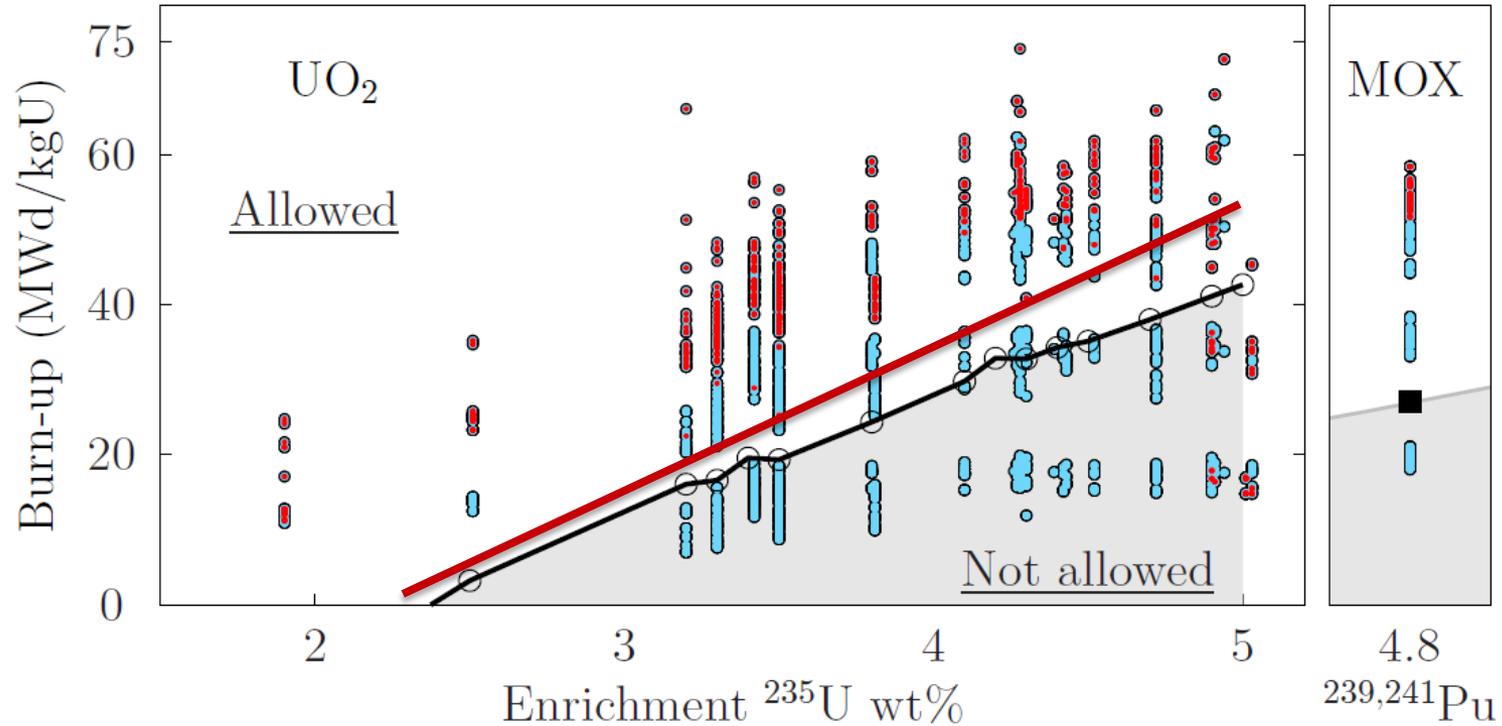


Fig. 6. Loading curve calculated with $k_{\text{eff}} = 0.95$, taking into account all assembly-cycles. The lines denotes the limit between the allowed and not allowed zones for the canister loading with 4 identical assemblies. The blues dots are all the assembly-cycles considered (assemblies being discharged or reloaded) and the red dots indicate the assemblies used in their last cycles.

- Criticality calculations, where is the limit ?



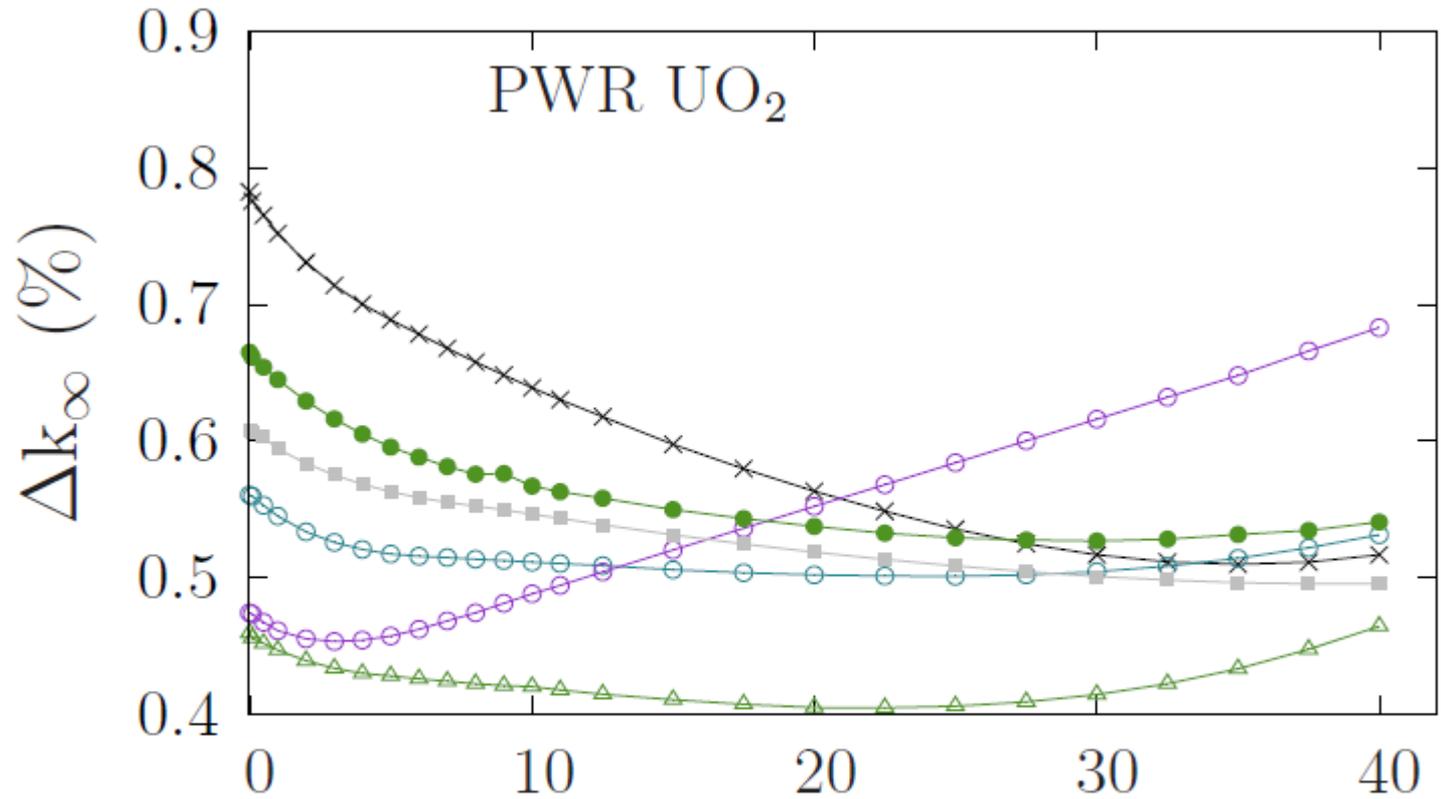
— Example of the impact of the nuclear data uncertainties on the loading curve:
less assemblies → more expensive storage !!

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).

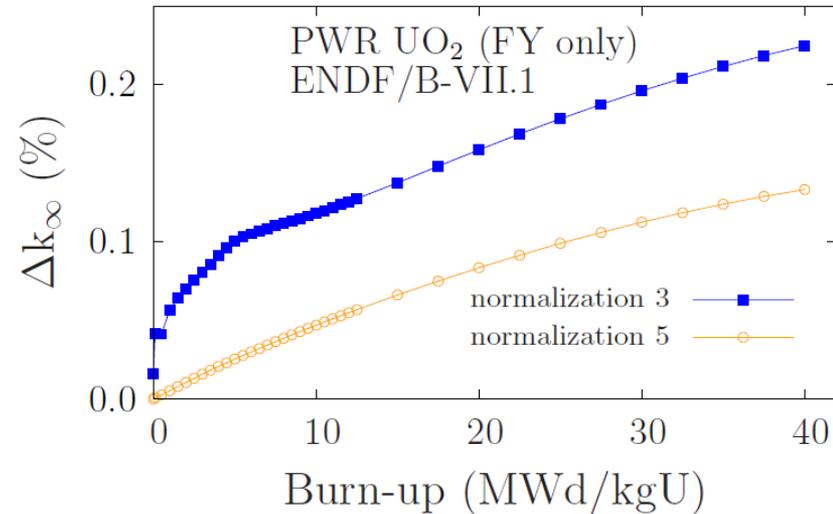
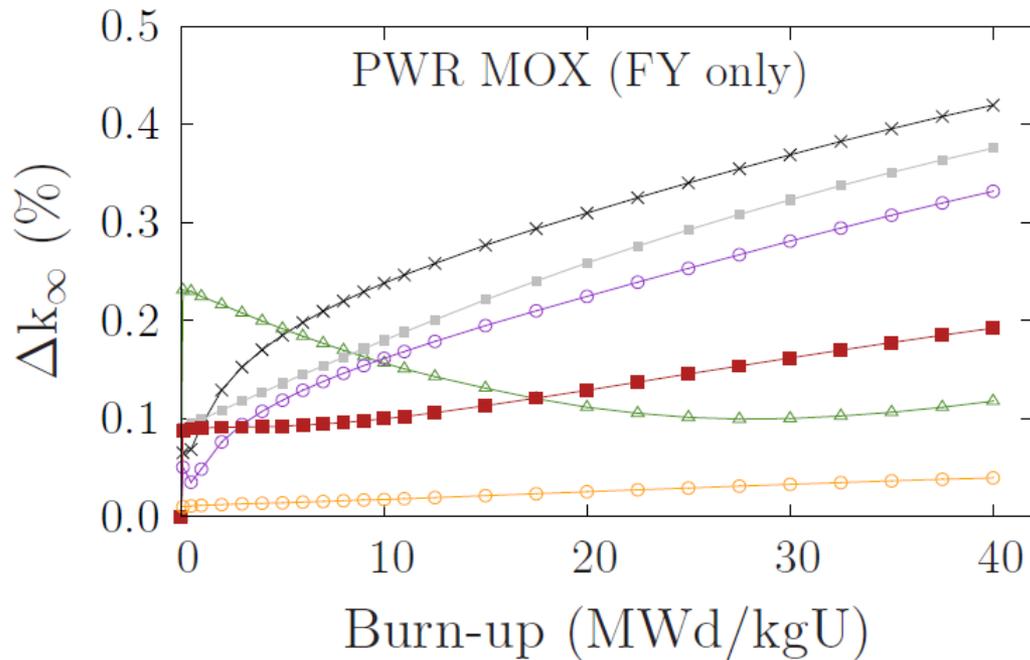
Uncertainty from methods



- CASMO + ENDF/B-VII.1 (PSI) — × —
- CASMO + SCALE-6.2 (PSI) — ○ —
- DRAGON + JENDL-4.0 (UU) — ▲ —
- DRAGON + ENDF/B-VII.1 (UU) — ● —
- TRITON + SCALE-6.1 (GRS) — ○ —
- TRITON + SCALE-6.2 (UPM) — ■ —

Burn-up (MWd/kgU)

Uncertainty from methods



- GEF — x —
- ENDF/B-VII.1 normalization 1 — Δ —
- ENDF/B-VII.1 + normalization 2 — ■ —
- ENDF/B-VII.1 + normalization 3 — ○ —
- ENDF/B-VII.1 + normalization 4 — ■ —
- ENDF/B-VII.1 + normalization 5 — ○ —

- Normalization 1: mass & charge
- Normalization 2: GEF correlation
- Normalization 3: Updated GEF (see [1])
- Normalization 4: $\Sigma_{FY=2}$
- Normalization 5: SANDY

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

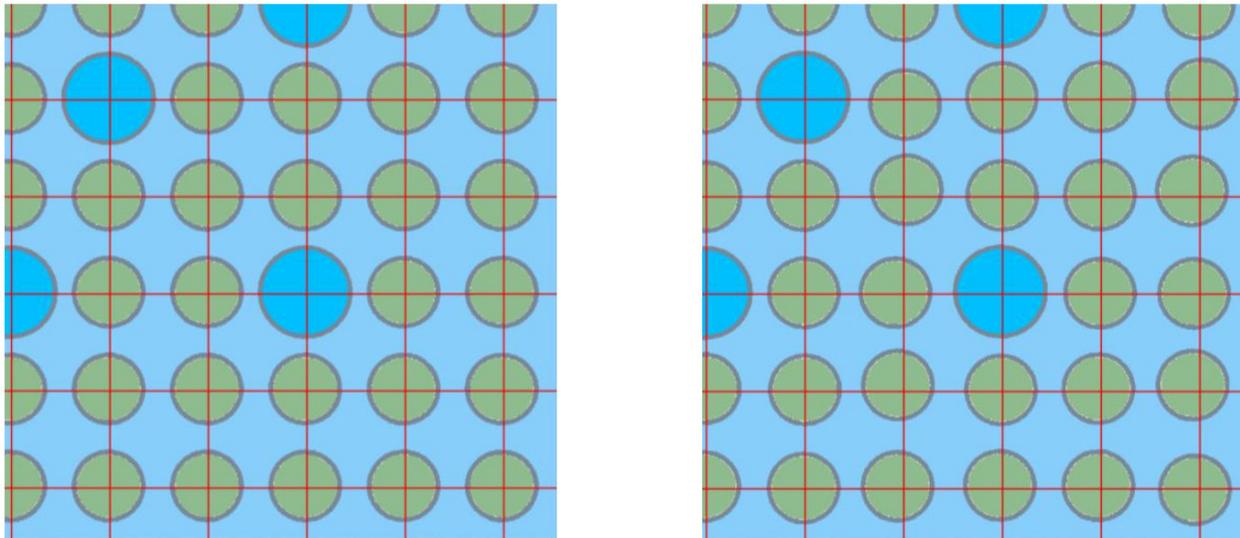
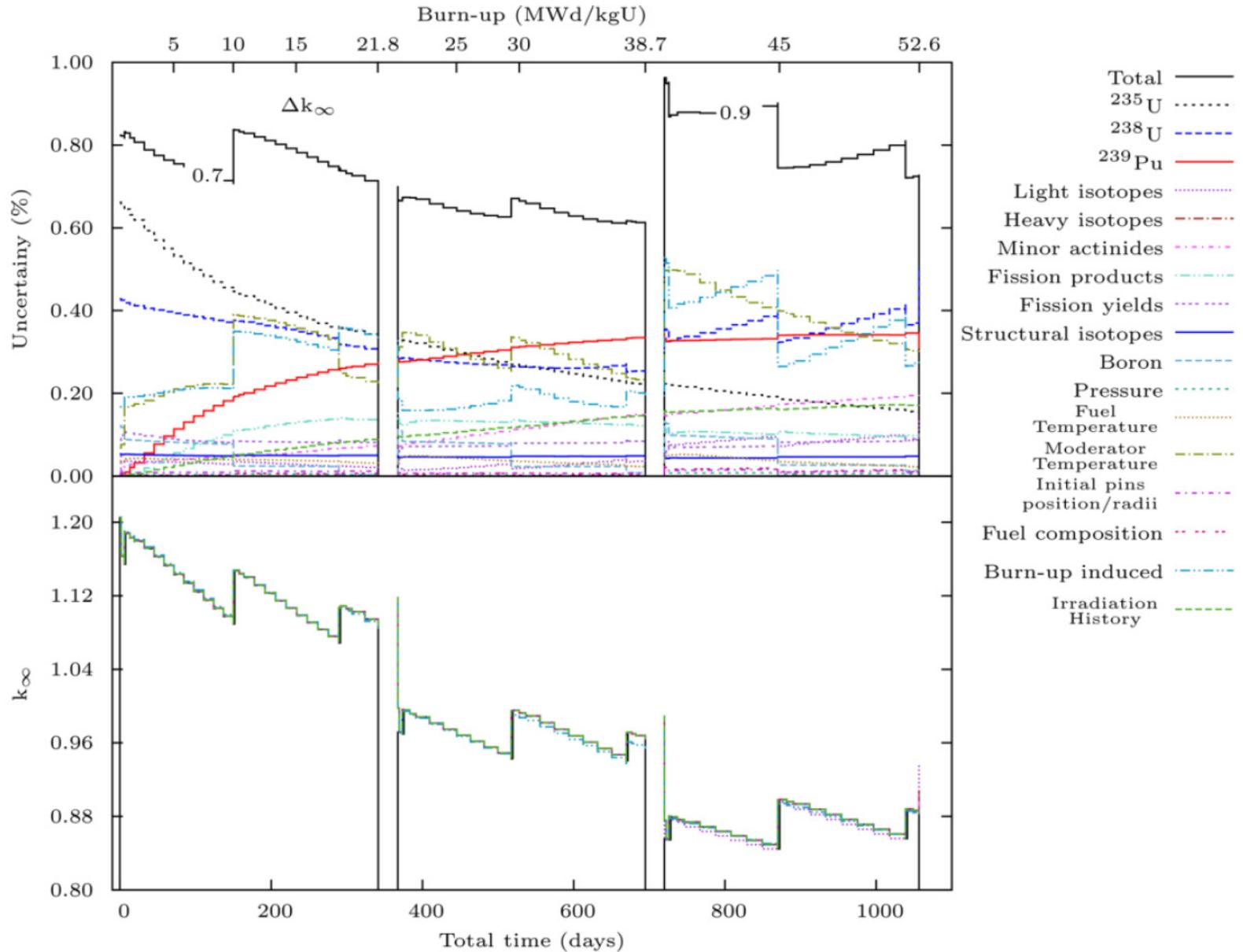


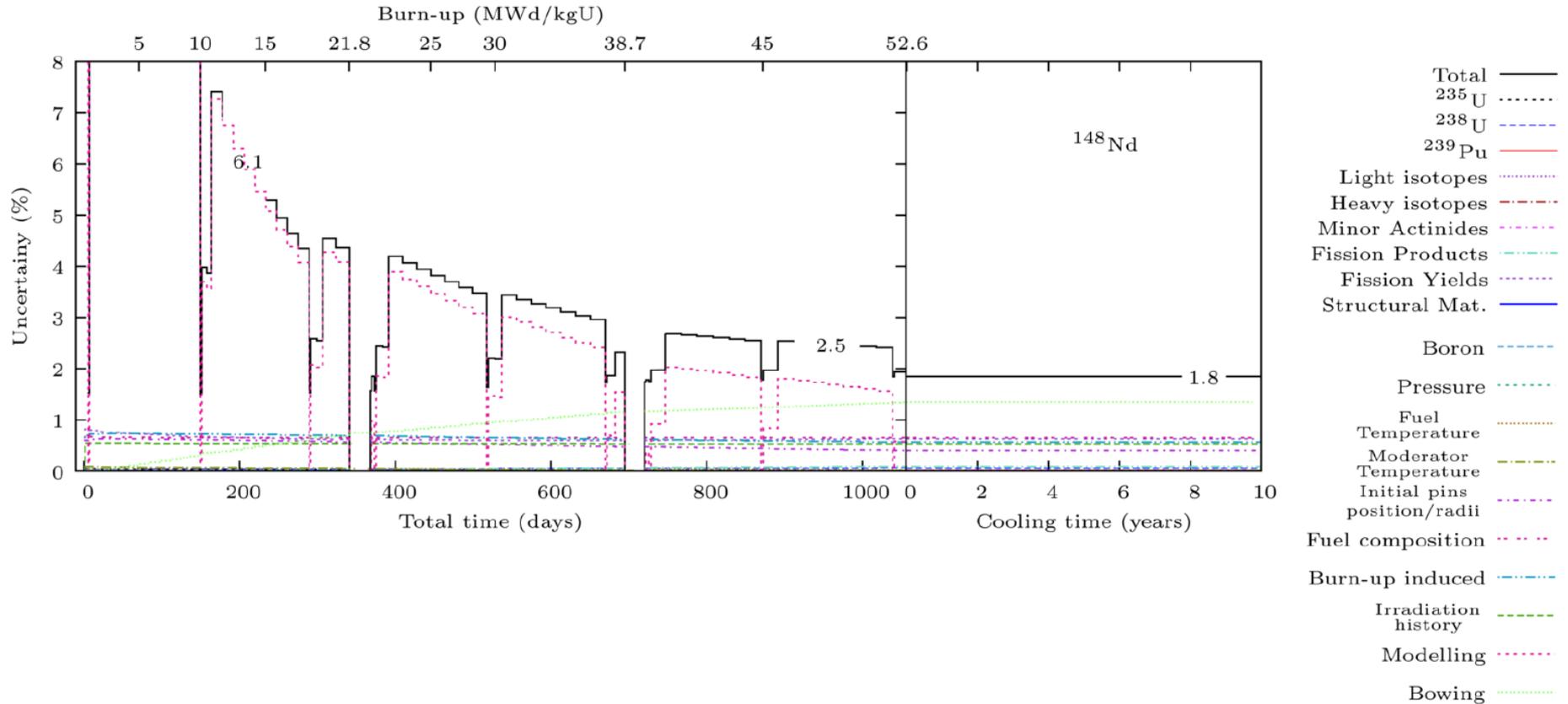
Figure 9:

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

Other Uncertainties

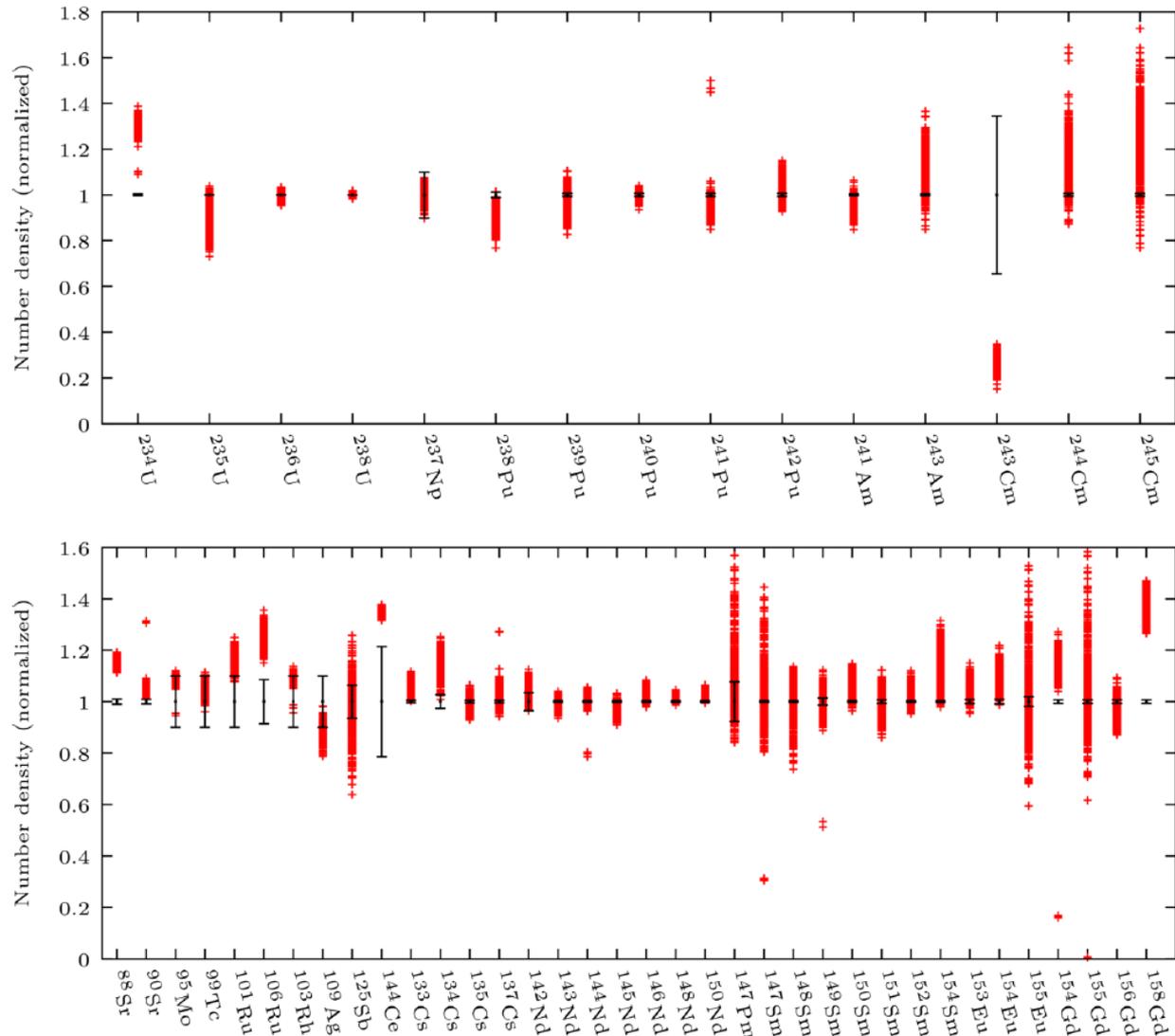


Other Uncertainties



Other Uncertainties

- Finally, the analysis of the total uncertainties help to explain possible differences in C/E ratios



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



$^{238}\text{U}(n, \text{inl})$ and nonlinearity in PWR core safety parameters

$^{238}\text{U}(n,\text{inl})$: state of knowledge

- $^{238}\text{U}(n,\text{inl})$ is an important cross section in reactor applications (LWR and fast systems),
- $^{238}\text{U}(n,\text{inl})$ is known with a relative poor accuracy: 20% from 1 to 5 MeV,
- 95 % of the fuel in LWR is made of ^{238}U ,
- The fast neutron population in a LWR is affected by this cross section.

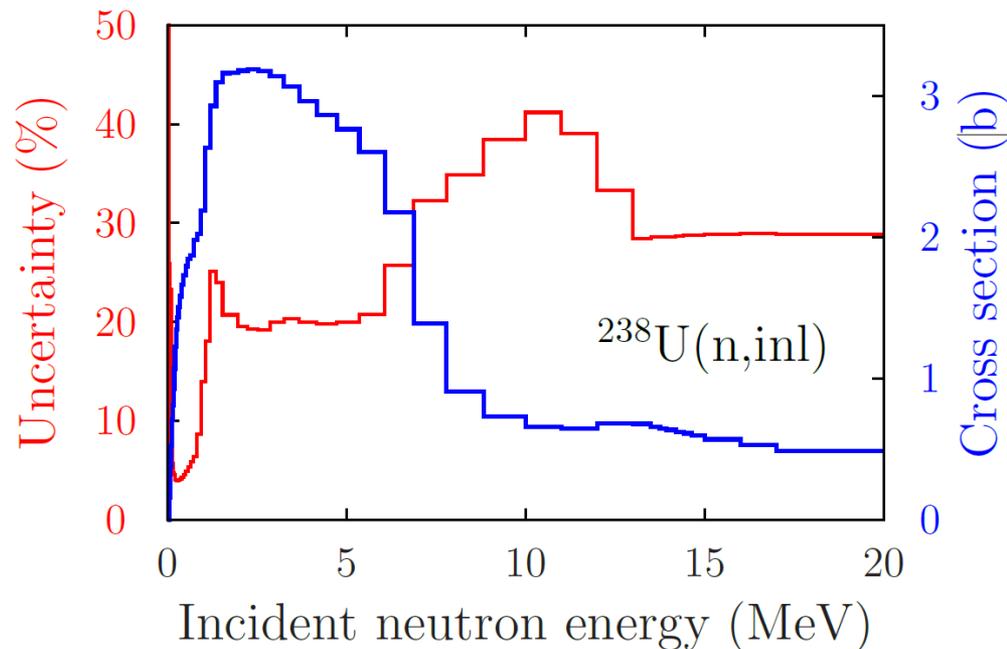
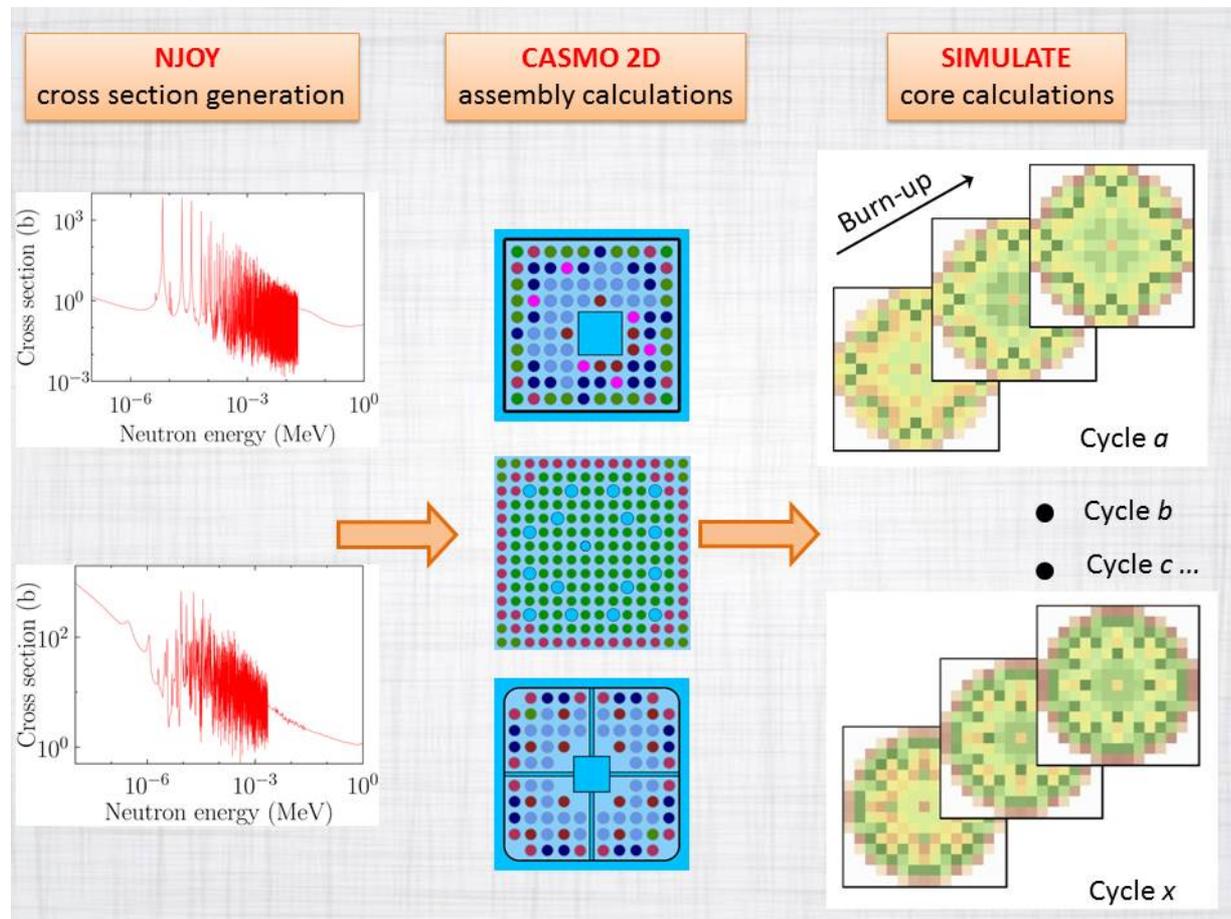


Fig. 1 Inelastic cross section and uncertainties for ^{238}U from the ENDF/B-VII.1 library. Left Y-axis: uncertainties, right Y-axis: cross section.

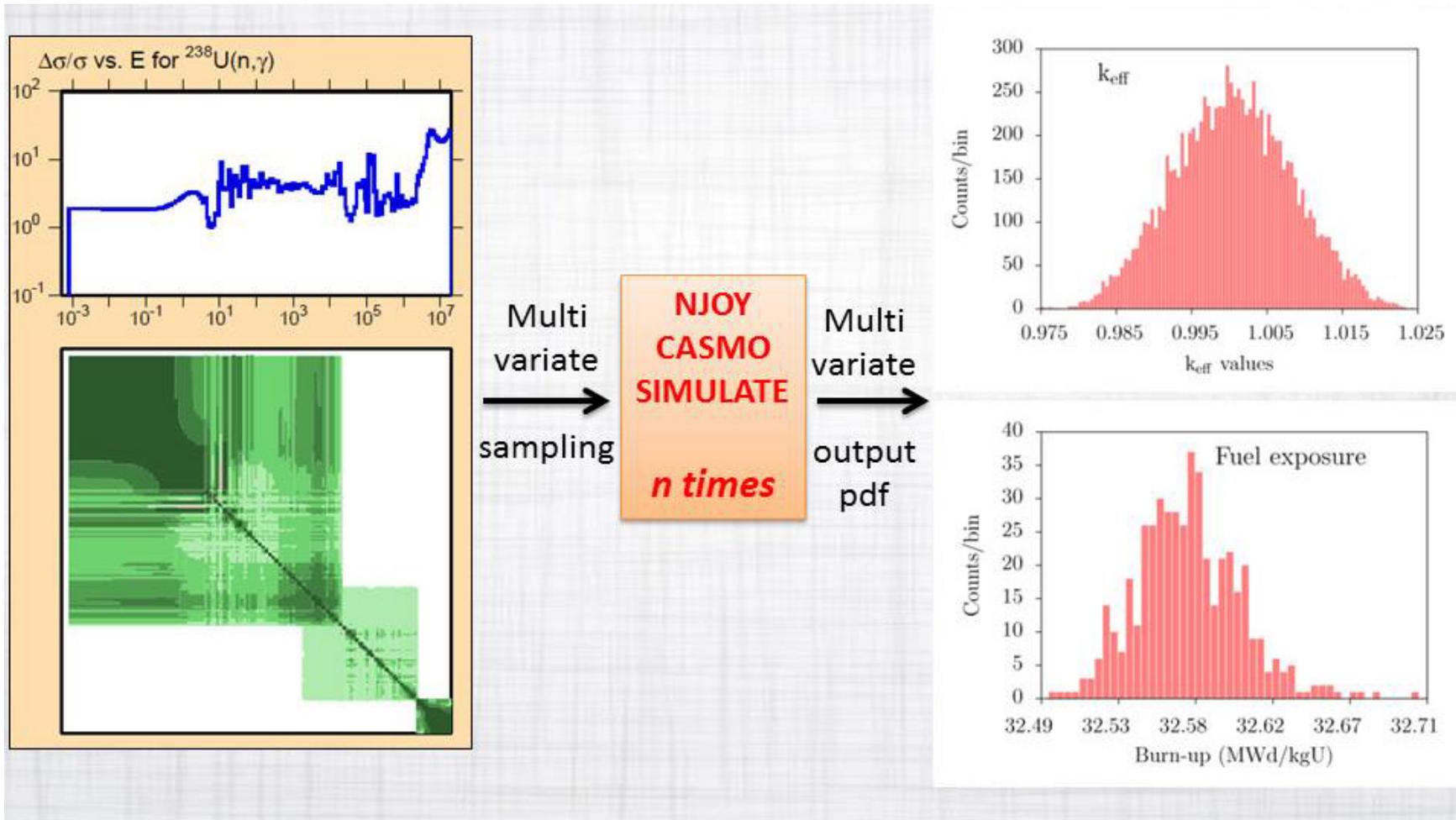
Reactor cycle calculation: state of the art

- At PSI, we have access to the core history for a number of LWRs,
- Power, fuel types, cycles, shutdown, temperatures, fuel shuffling, measurements,
- This covers decades of service,
- We have developed validated models based on commercial lattice and full core codes



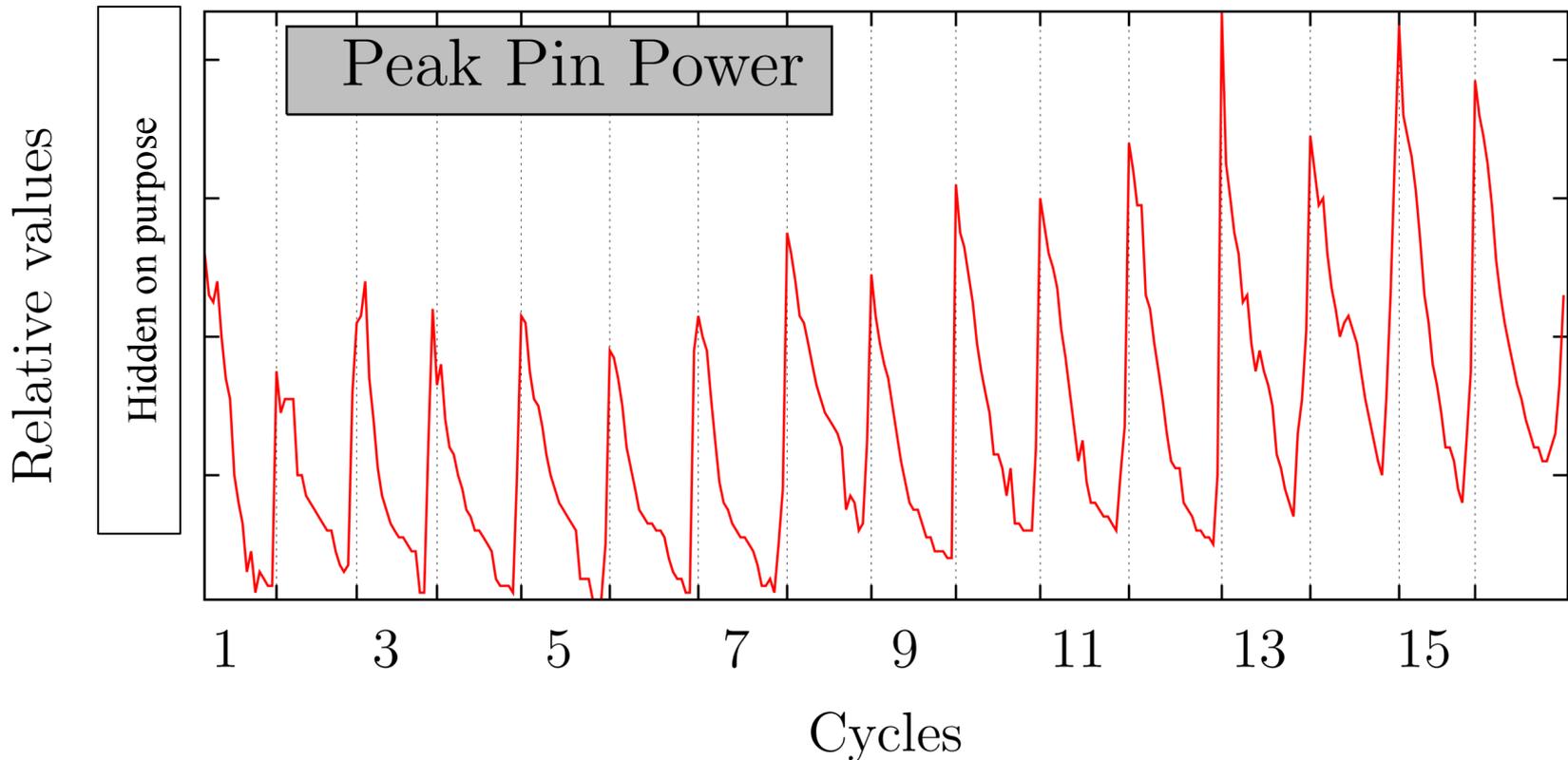
Nuclear data uncertainties: from covariances

- For the core follow-up calculations, we have developed capabilities to vary the nuclear data,
- The module/code SHARK-X uses existing covariance files and generate random cross sections,
- For this work, the ENDF/B-VII.1 library is used.
- Uncertainty propagation: simple TMC-like.



Important core parameter

- We will focus in the following in one core parameter for simplicity,
- The so-called “**peak pin power**” (ppp) is a safety relevant parameter,
- It represents the maximum local power in the 3D core at a specific running time,
- In core licensing, the ppp needs to stay below a limit.



Important core parameter

- The ppp is position and time dependent (x,y,z,t) : max of the pin power (pp)
- The pin power also depends on the $^{238}\text{U}(n,inl)$ cross section:
 - For the pp close to the center:
 - $^{238}\text{U}(n,inl)$ **decrease** → fast neutron flux increase → leakage increase → more neutrons at the center → peaked power map at the core center → pp **increase**
 - For the pp close to the core side:
 - $^{238}\text{U}(n,inl)$ **decrease** → fast neutron flux increase → leakage increase → more neutrons at the center → decrease of power in the core side → pp **decrease**

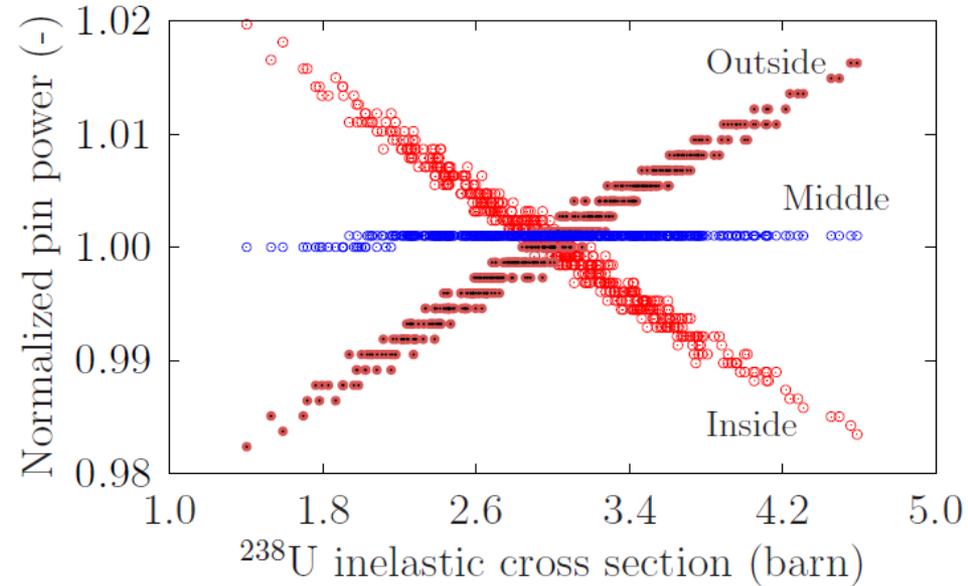
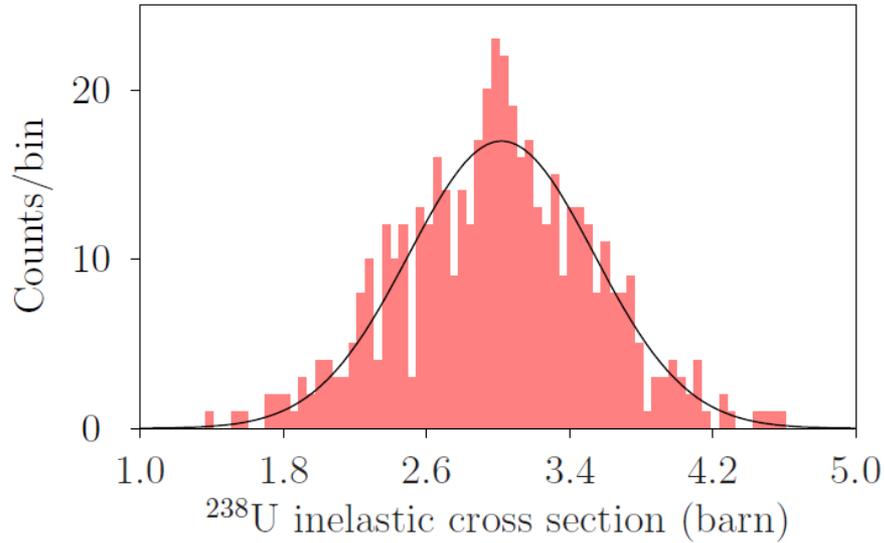
- Therefore,

$$\begin{aligned}
 ppp &= \max(pp) \\
 &= \max \left[fct \left(^{238}\text{U}(n,inl) \right) \right]
 \end{aligned}$$

is increasing or decreasing depending on its core position

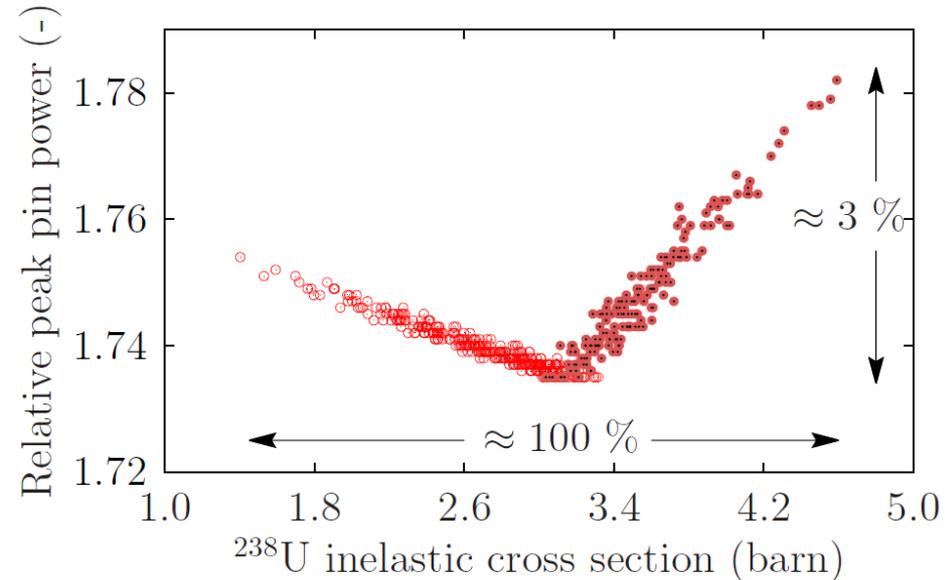
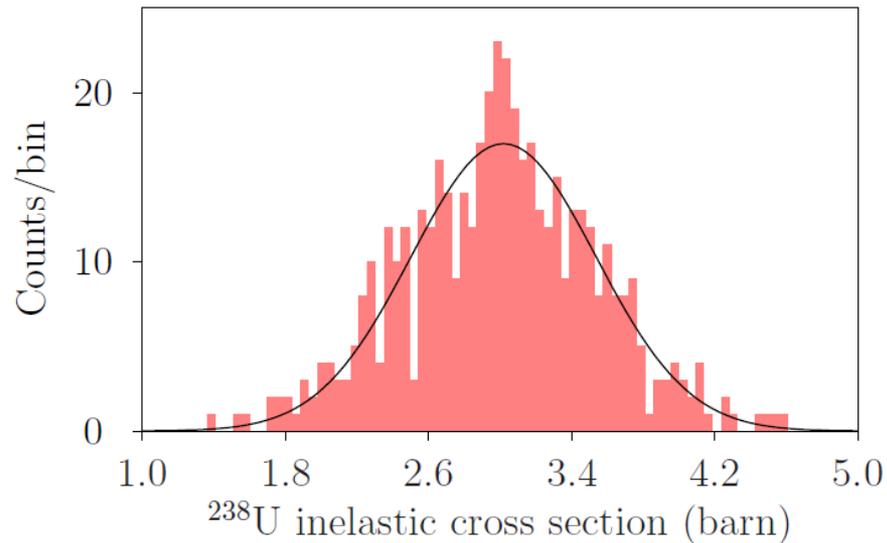
Important core parameter: **pin power**

- Example of the variation of pp (pin power, not the max !)



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 $^{238}\text{U}(n,\text{inl})$, 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 $^{238}\text{U}(n,\text{inl})$ (20% from 1 to 5 MeV)

Conclusion

- Current knowledge on $^{238}\text{U}(n,\text{inl})$ is 20 % uncertainty from 1 to 5 MeV,
- Based on ENDF/B-VII.1 and real PWR history, the peak pin power becomes nonlinear as a function of $^{238}\text{U}(n,\text{inl})$,
- Not presented here, but $^{238}\text{U}(n,\text{inl})$ affects many other quantities,
- Solution: lower the uncertainty from 20 to 10 %,
- Open questions:
 1. is it possible ?
 2. Other core type (BWR) ?
 3. Other pdf (from TMC) ?
- Publication under preparation.

