TMC vs. perturbation

and other applications

D. Rochman and A.J. Koning

Nuclear Research and Consultancy Group,

NRG, Petten, The Netherlands

Uppsala TMC meeting, April 2013

Contents

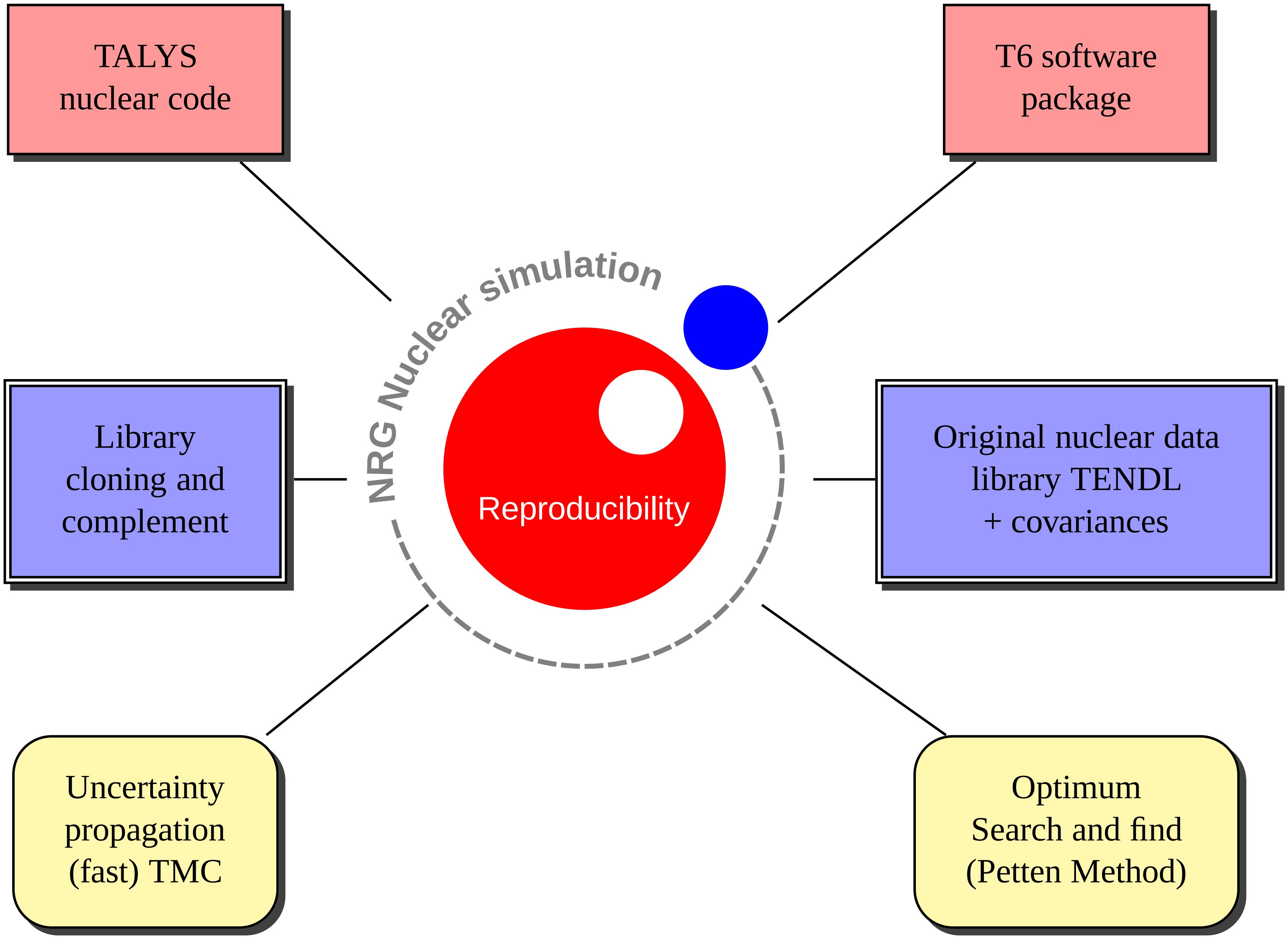
All slides can be found at:
ftp://ftp.nrg.eu/pub/www/talys/bib_rochman/presentation.html.

Introduction to nuclear data uncertainties

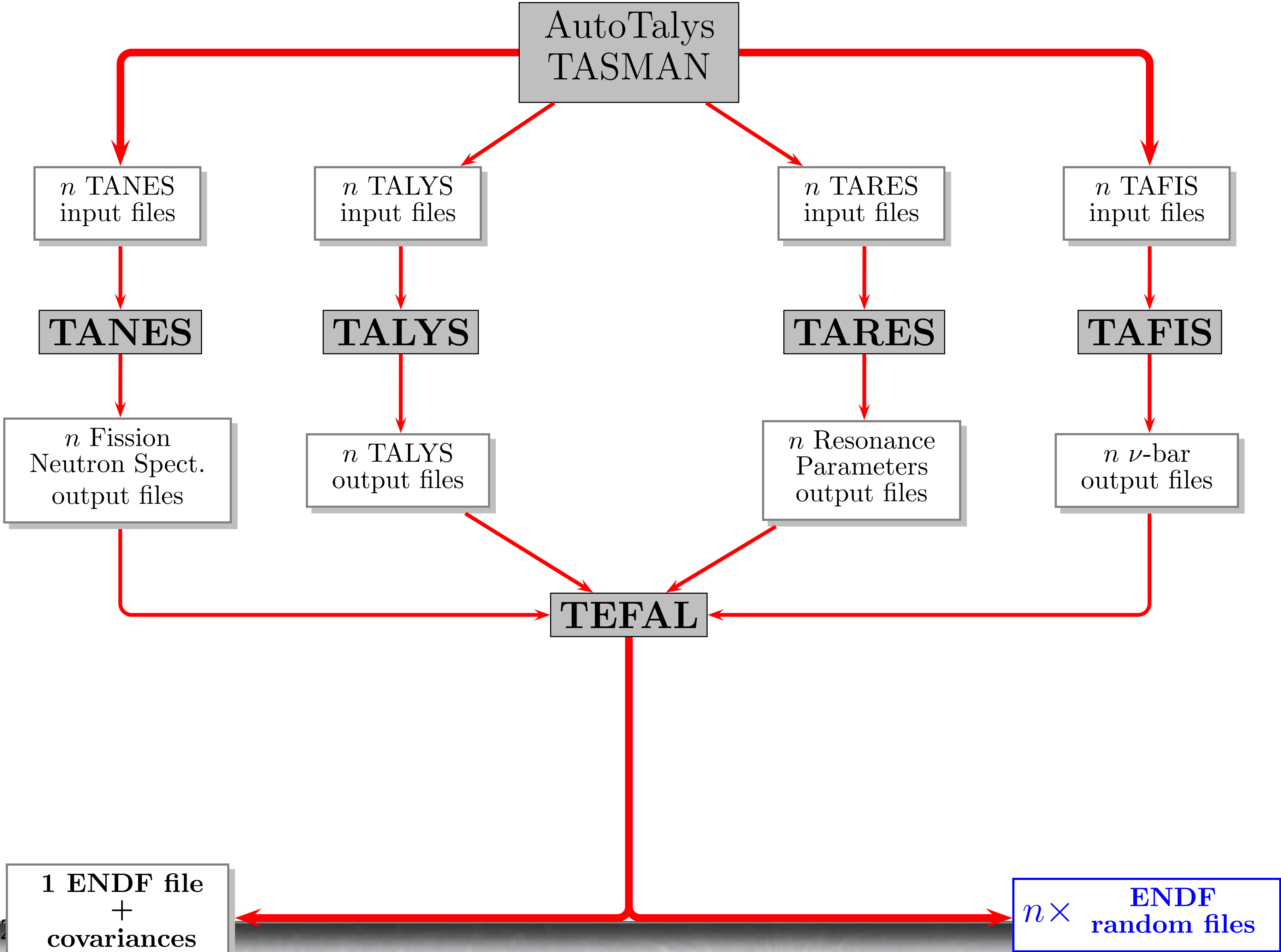
General comments:

- uncertainties are not errors (and vice versa),
- uncertainties should now be given with all data (seems obvious ?),
- they are related to risks, quality of work, money, perception, fear, safety...
- Uncertainty $\leftrightharpoons$ safety $\leftrightharpoons$ 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 !

Backbone of our methodology: REPRODUCIBILITY



TMC: procedure for the random file production



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...)

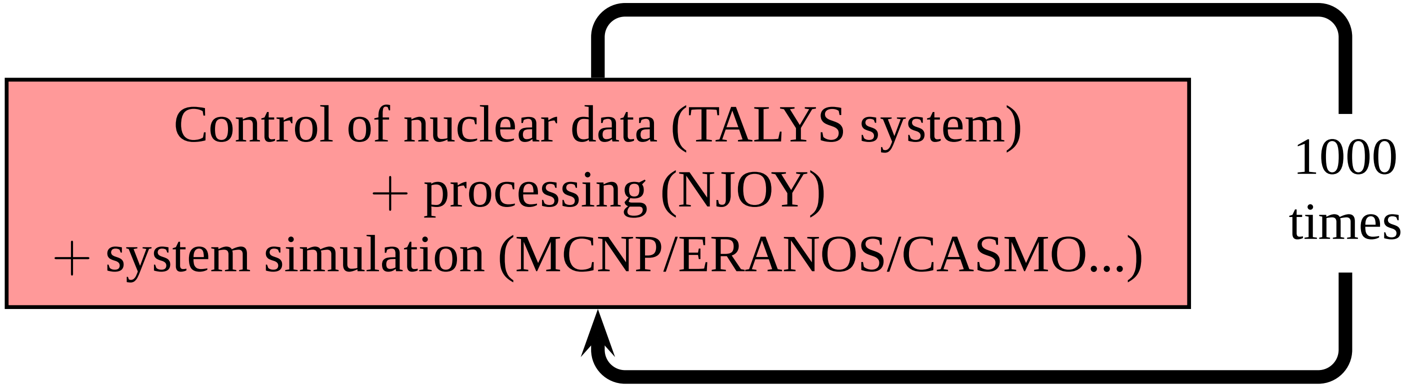
☺ + QA.

☹ - Needs discipline to reproduce,

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

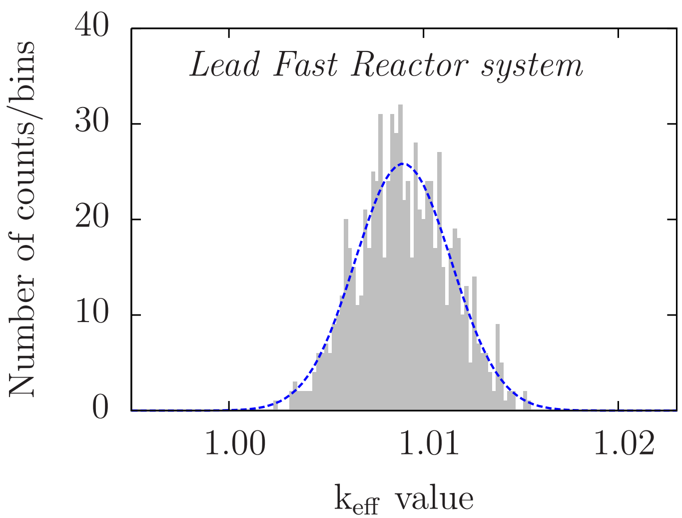
☹ - Need mentality change.

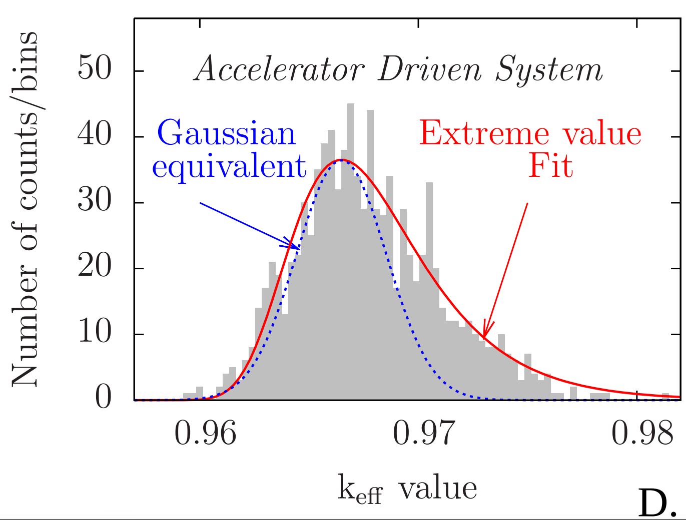
2008: Total Monte Carlo (TMC)



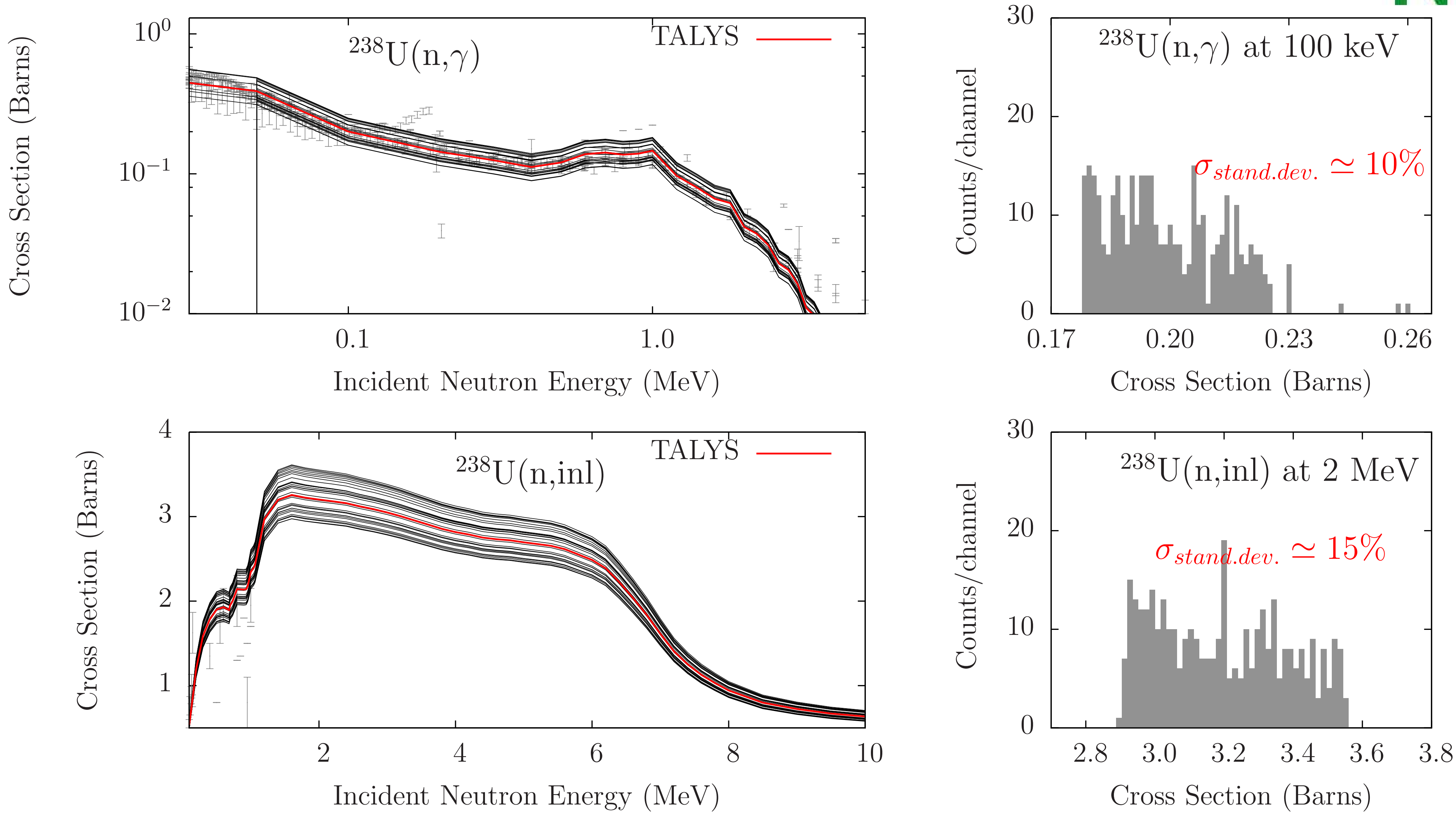
For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the *n* calculations, *n* different k_{eff} values are obtained.

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

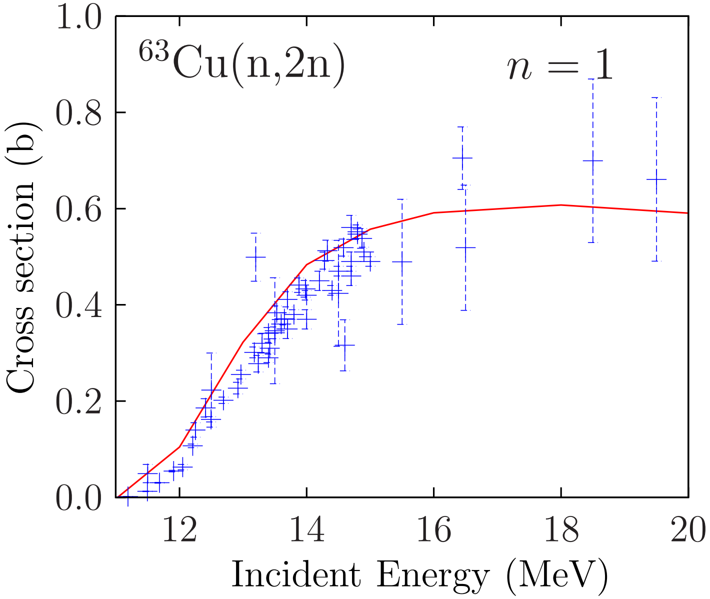


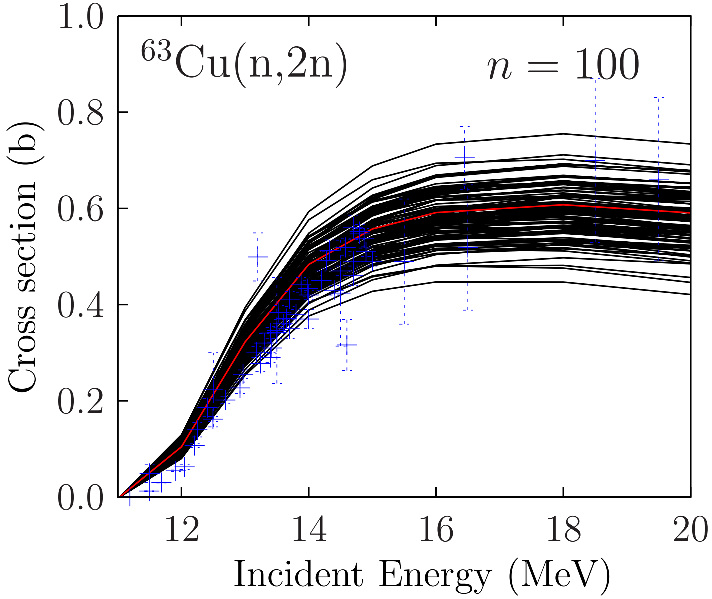


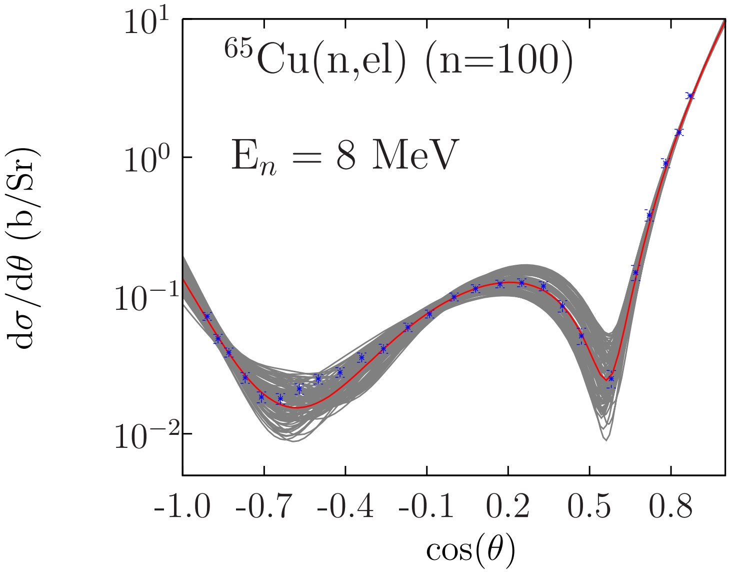
Example with ^{238}U: Monte Carlo calculations

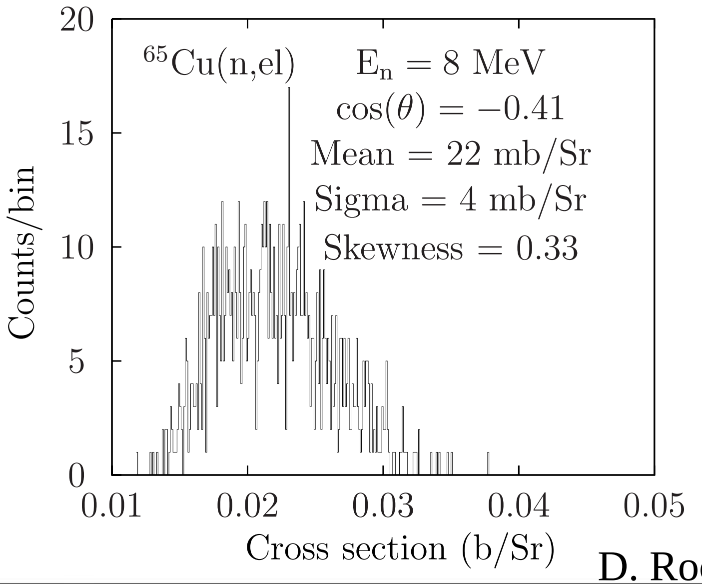


Examples with ^{63}Cu(n,2n) and ^{65}Cu(n,el)

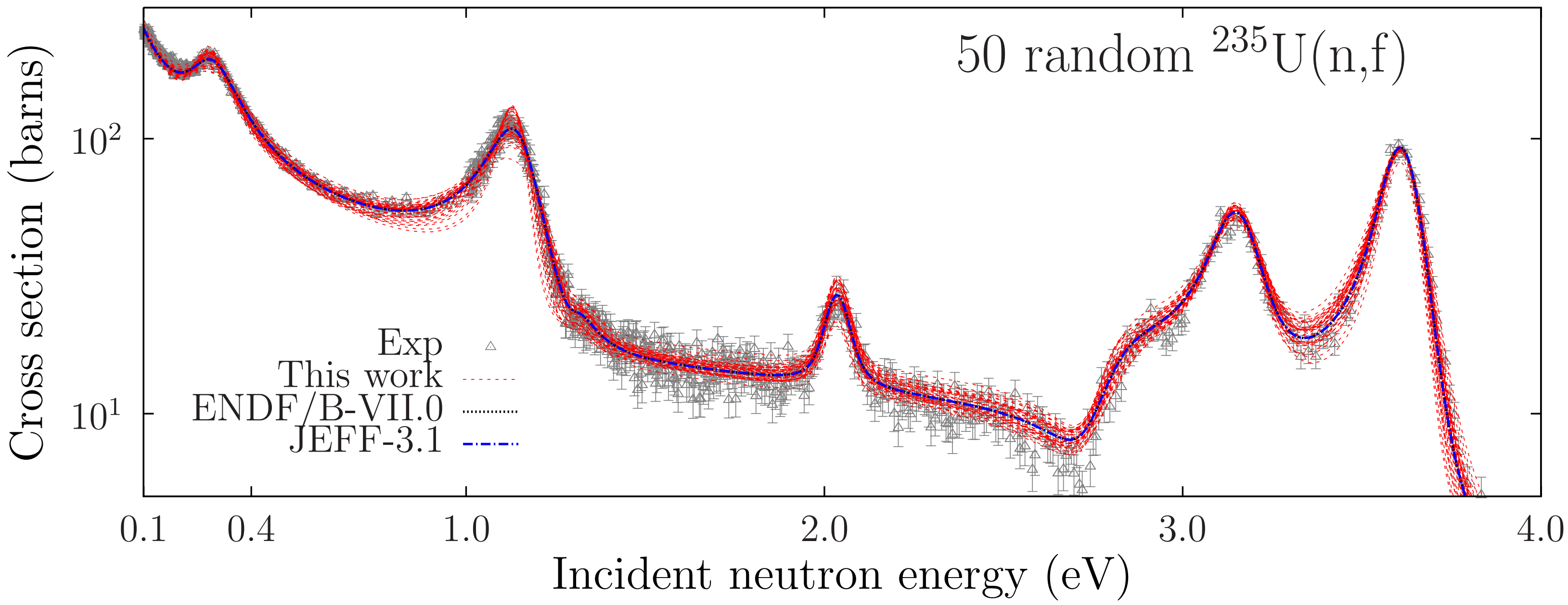


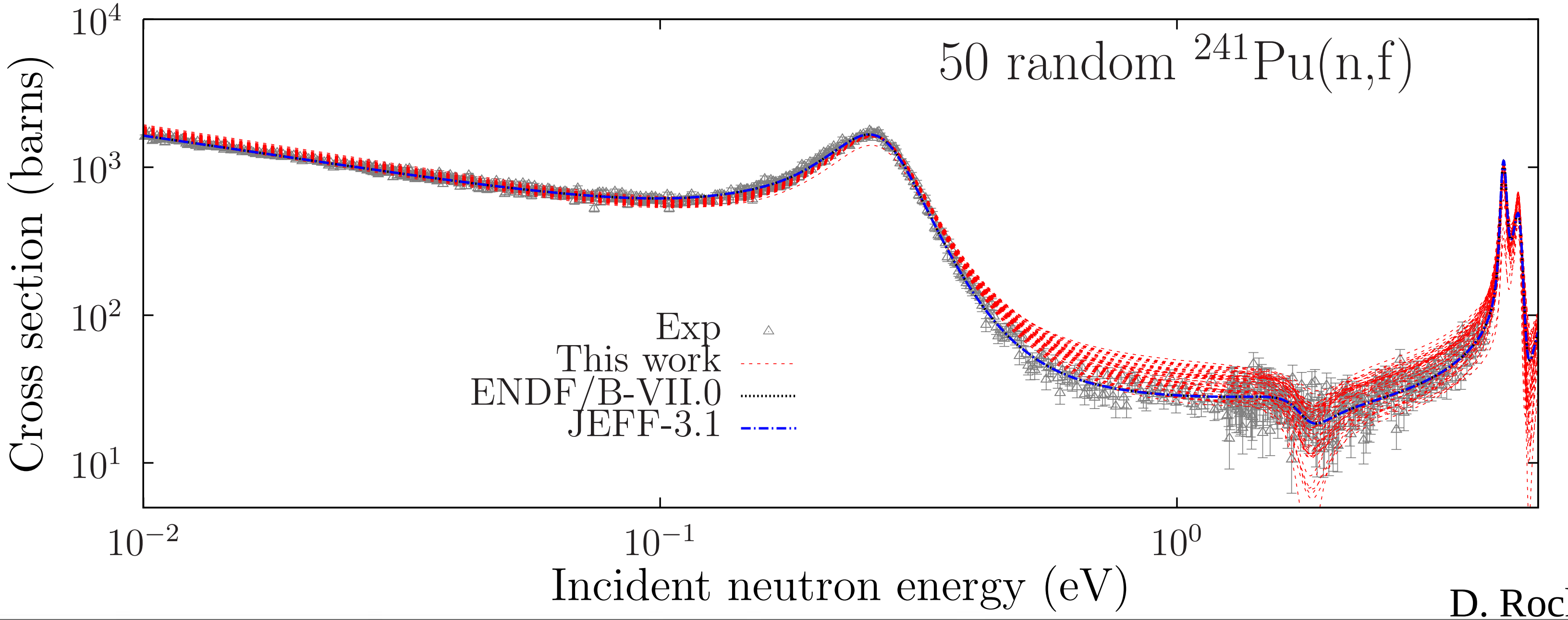






Nuclear data: examples in the resonance region



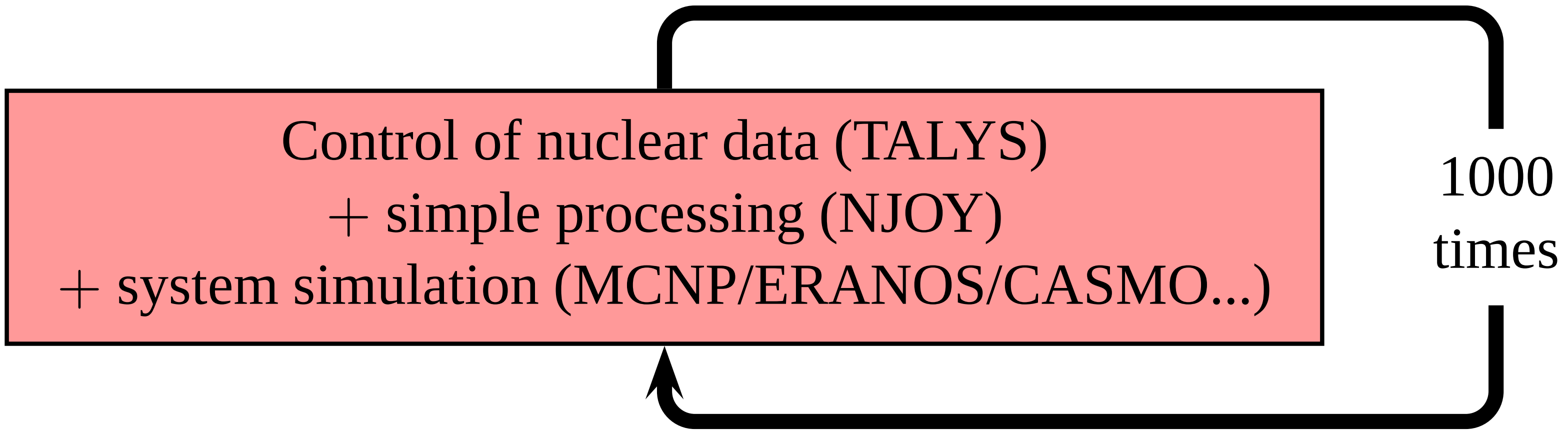


TMC versus Perturbation method

① Obtain uncertainties on large-scale models due to nuclear data uncertainties

② Systematic approach, reliable and reproducable

Solution (1): Total Monte Carlo



Solution (2): Perturbation method

$\Longrightarrow$MCNP+ Perturbation cards+covariance files

TMC versus Perturbation: Results

Comparison TMC-Perturbation methods for a few k_{eff} benchmarks. The ratio in the last column is ”TMC over Perturbation”.

		Total Monte Carlo	Perturbation	Ratio
Benchmark	Isotopes	Uncertainty due to nuclear data (pcm)	Uncertainty due to nuclear data (pcm)	
hst39-6	^{19}F	330	290	1.16
hmf7-34	^{19}F	350	290	1.21
ict3-132	^{90}Zr	190	150	1.29
hmf57-1	^{208}Pb	500	410	1.22
pmf2	^{239}Pu	840	720	1.16
pmf2	^{240}Pu	790	650	1.21

Results: Details of the TMC-Perturbation methods for ^{239,240}Pu k_{eff} benchmarks

	pmf2 ^{239}Pu			pmf2 ^{240}Pu	
	Δk_{eff} (pcm)			Δk_{eff} (pcm)	
	TMC	Perturbation		TMC	Perturbation
Total	840	720		790	650
MF1	400	-		370	-
(n,inl)	170	140		70	50
(n,el)	250	240		30	40
(n,γ)	100	100		30	30
(n,f)	720	660		730	640
MF4	20	-		20	-
MF5	50	-		30	-
MF6	50	-		30	-

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,
- 2 Thermal scattering data: H in H_2O, D in D_2O
- 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

Considered data in TMC (or fast TMC)

Several hundreds of random ENDF files for transport + depletion

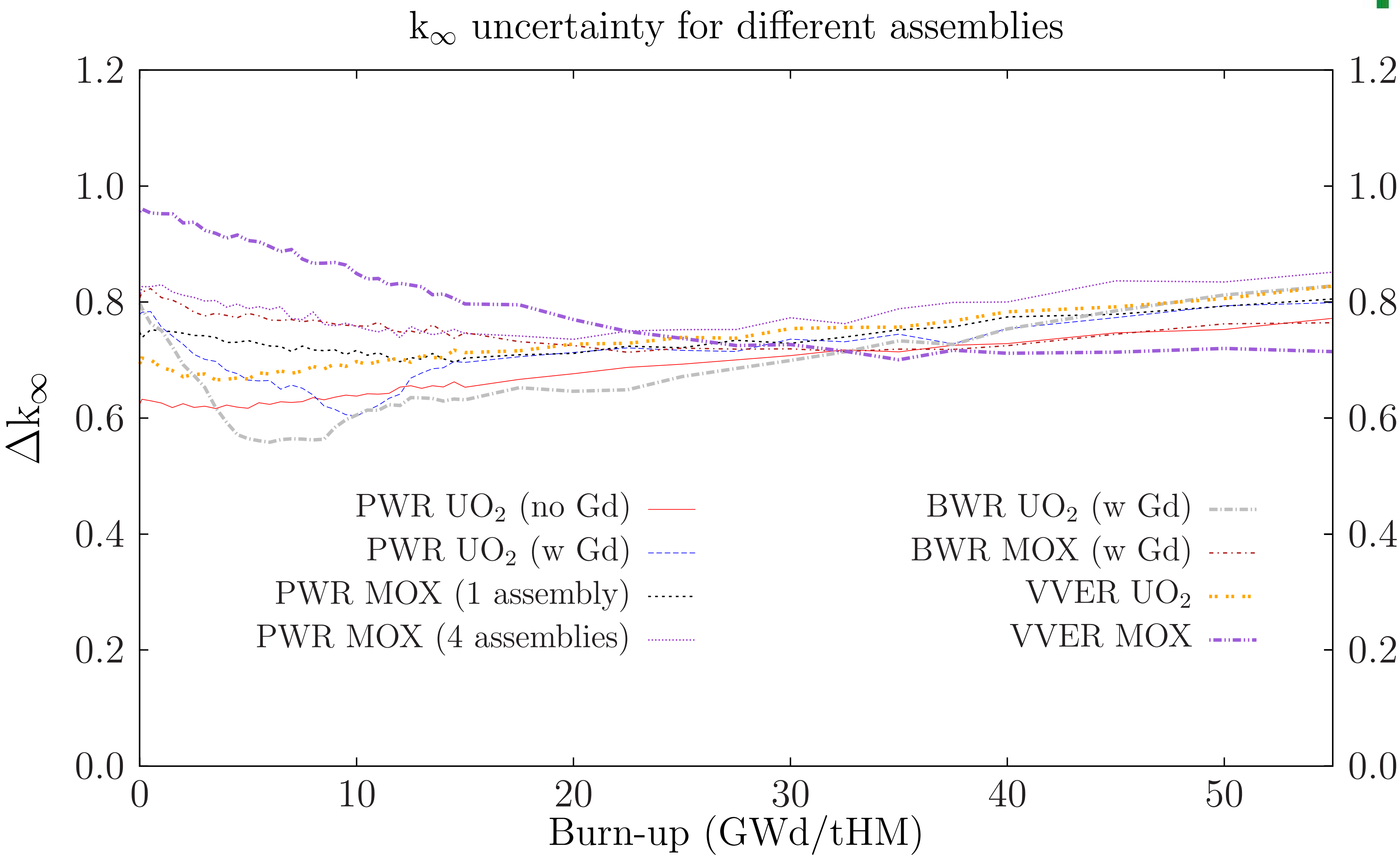
- 3 Major actinides: ^{235}U, ^{238}U, ^{239}Pu,
- Light elements: lighter than oxygen,
- 2 Thermal scattering data: H in H_2O, D in D_2O
- All Fission yields (e.g. ^{234,235,236,238}U, ^{239,240,241}Pu, ^{237}Np, ^{241,243}Am, ^{243,244}Cm),
- All Minor actinides (e.g. ^{234,236,237}U, ^{237}Np, ^{238,240,241,242}Pu,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

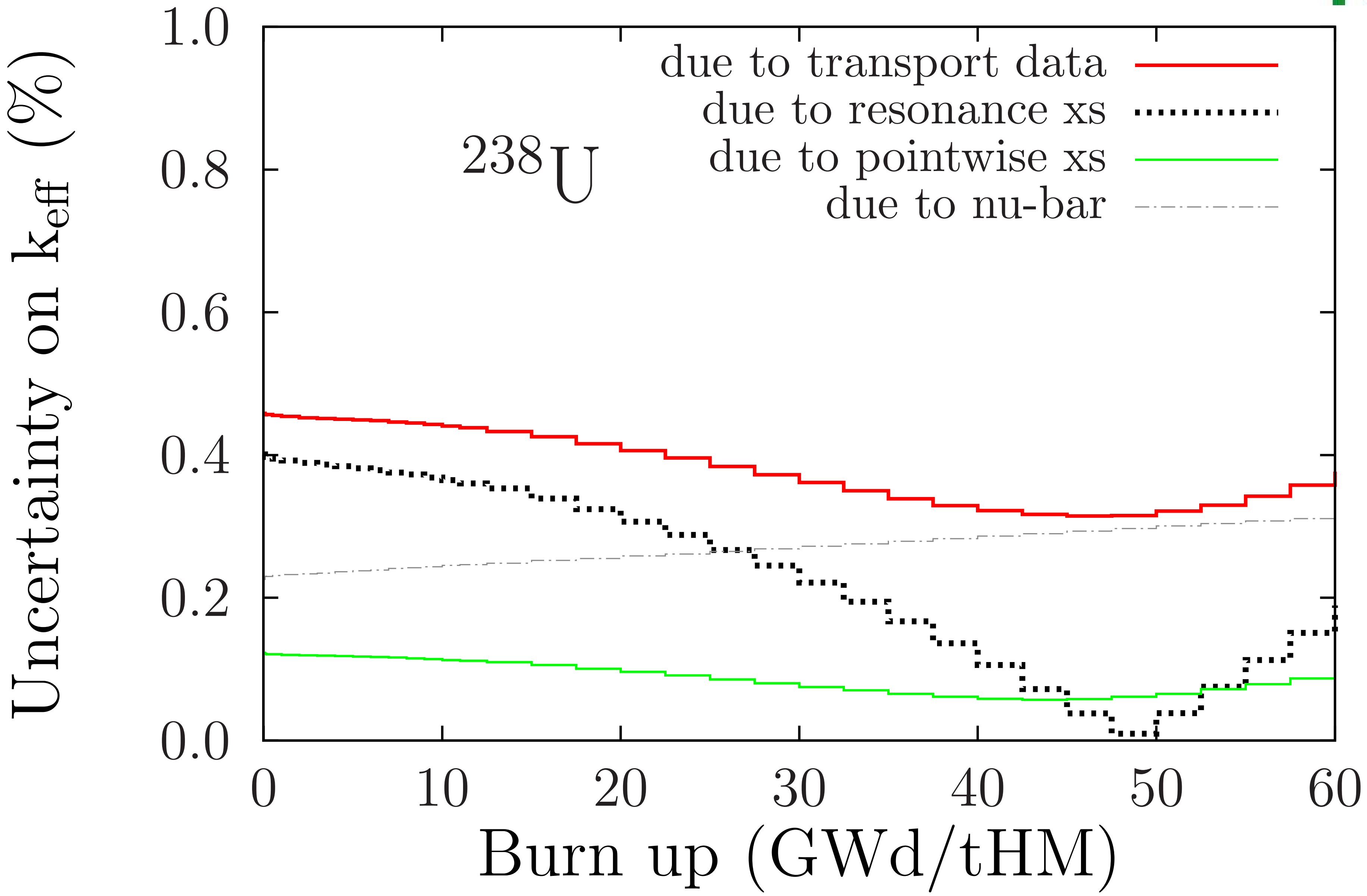
TMC was already applied to

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

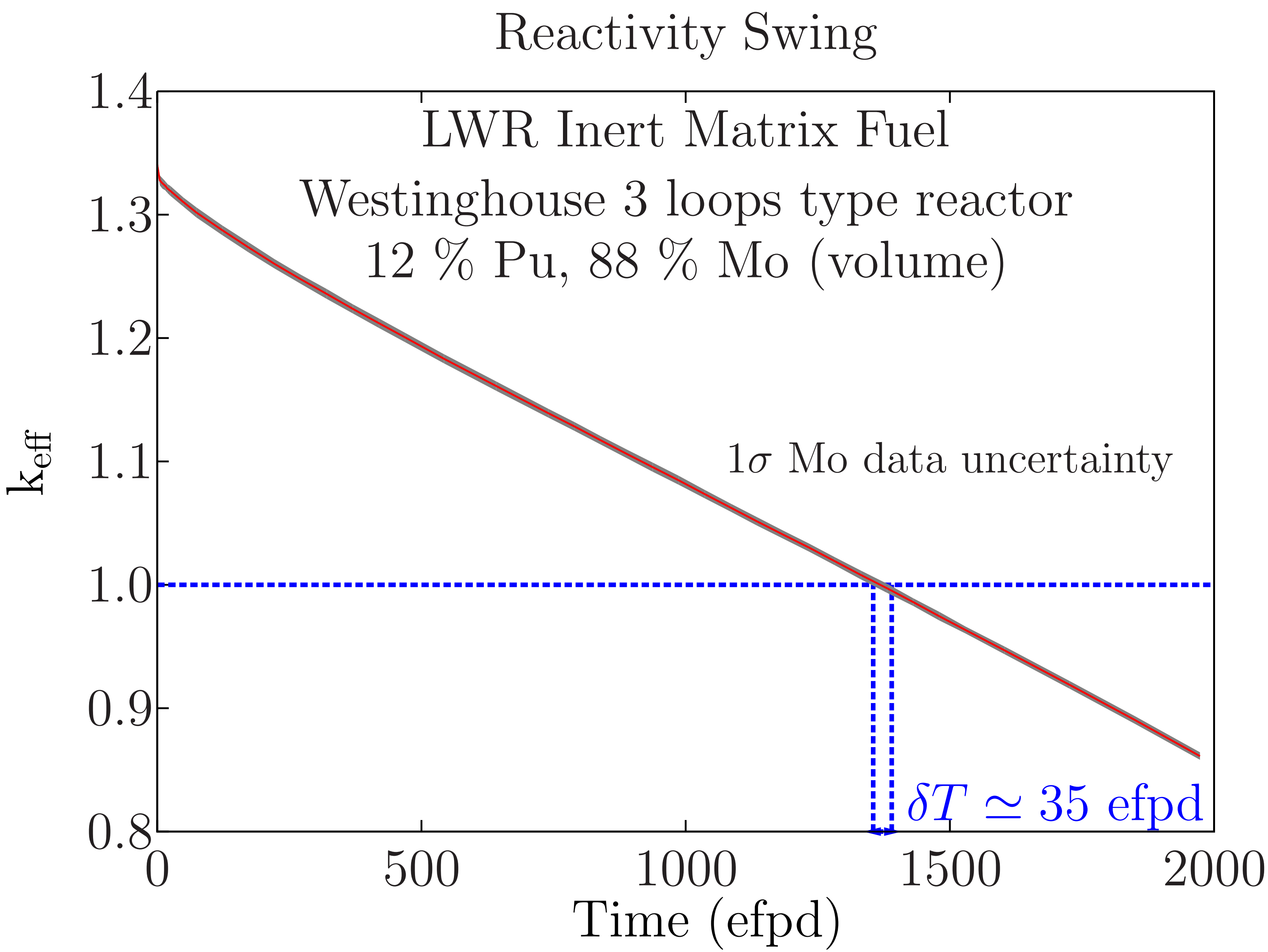
Comparison of Δk_∞ for assemblies and full core (SERPENT)



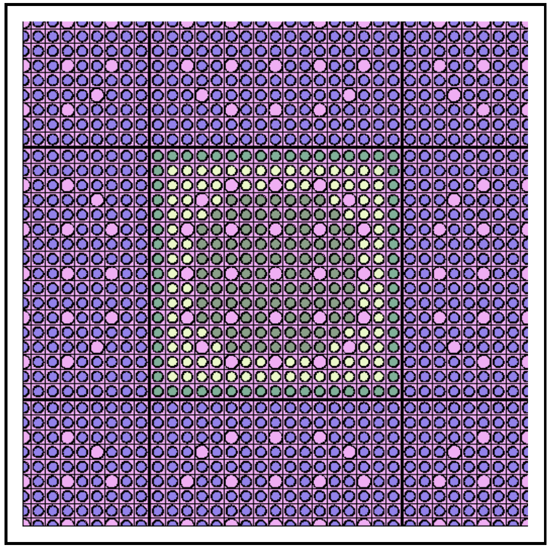
TMC applied to PWR assembly burn-up calculations with DRAGON

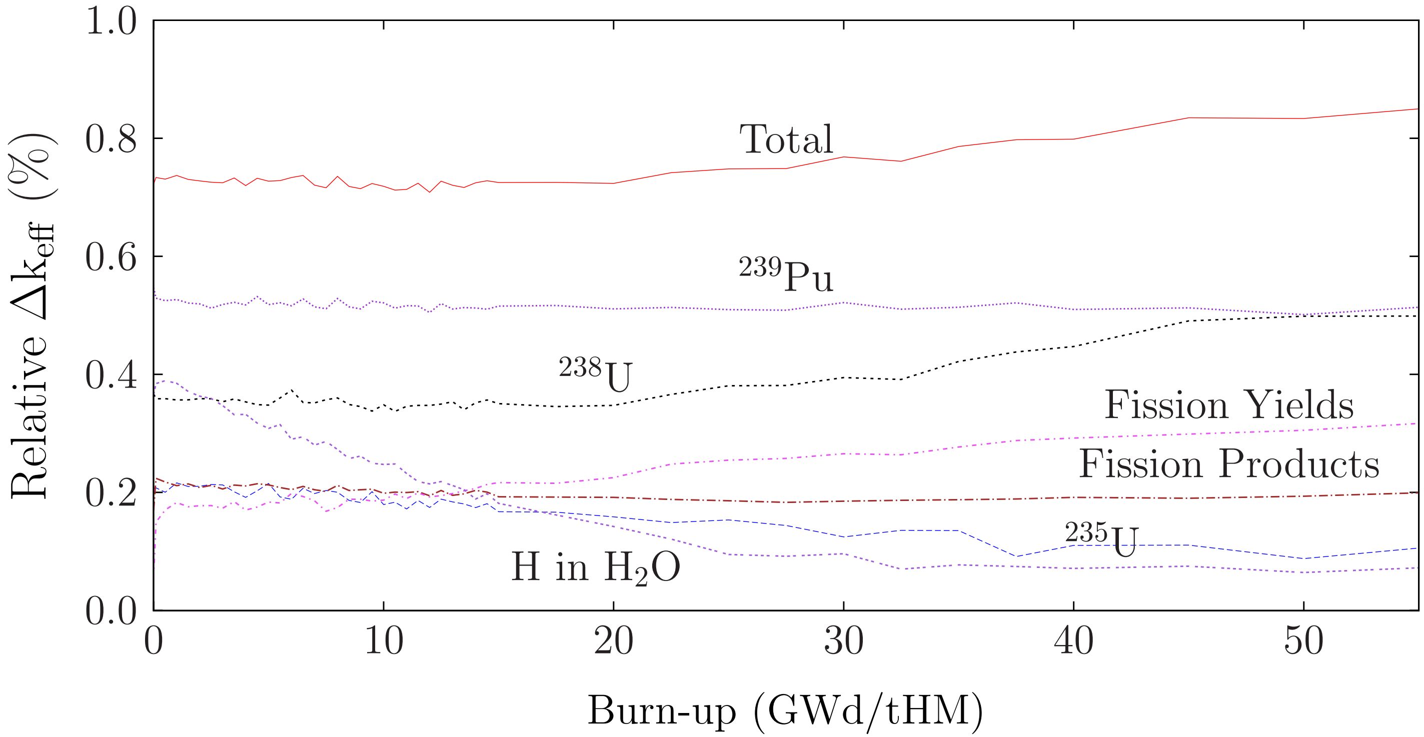


Example of TMC for the impact of the matrix fuel



PWR MOX assembly uncertainties





- 1 MOX assembly surrounded by UO_2 assemblies,
- Burn-up calculated with SERPENT,
- All major nuclear data taken into account.

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)

INDUSTRIALES ETSII | UPM

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						

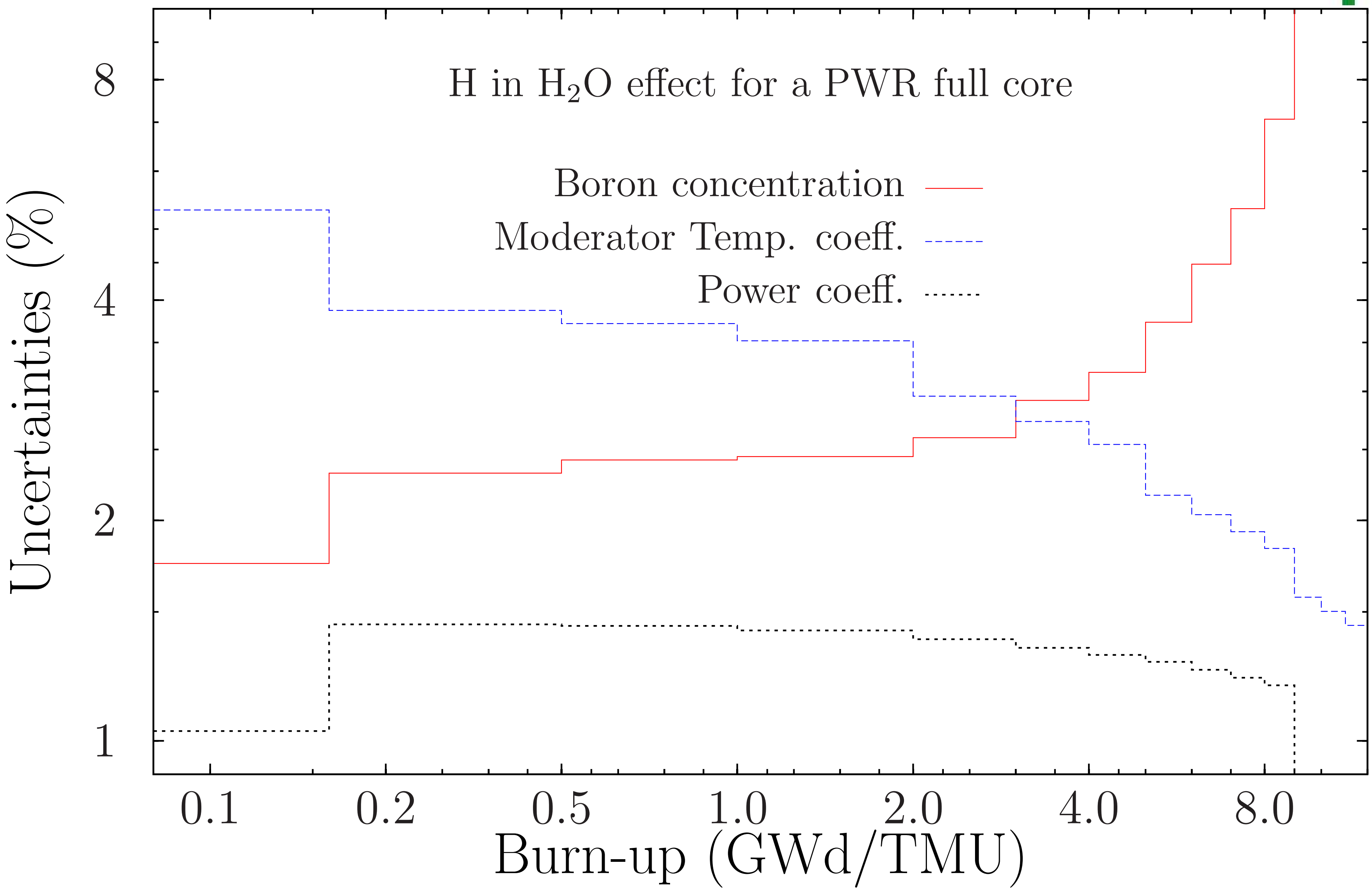
AVE. BURNUP PER FUEL ASSEMBLY

	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)



Drawbacks of the TMC method

In TMC:

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

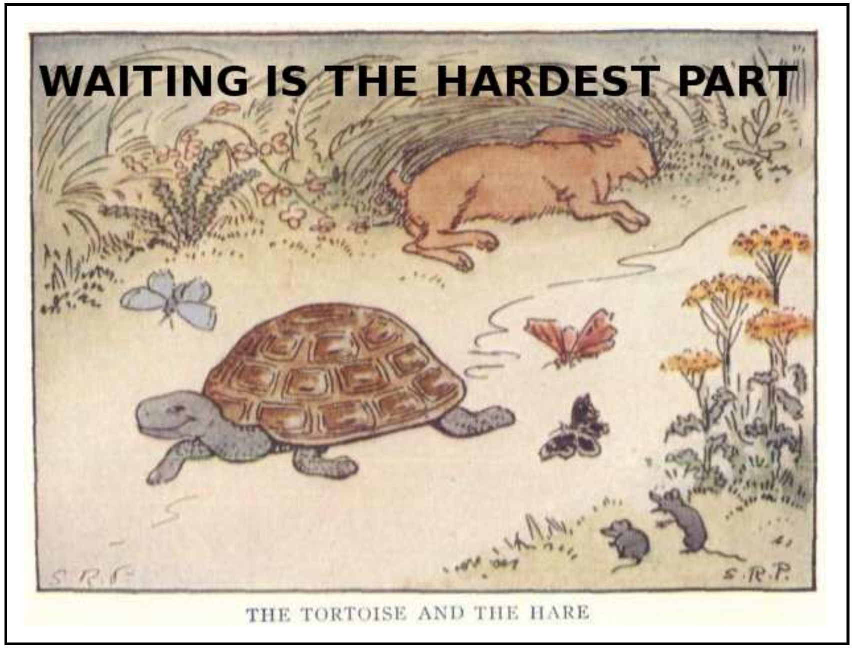
Drawbacks of the TMC method

In TMC:

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

Well, then uncertainty propagation with TMC takes 1000× longer than a single calculation...

(*Each* $\sigma_{\text{statistics}}$ *needs to be small*)

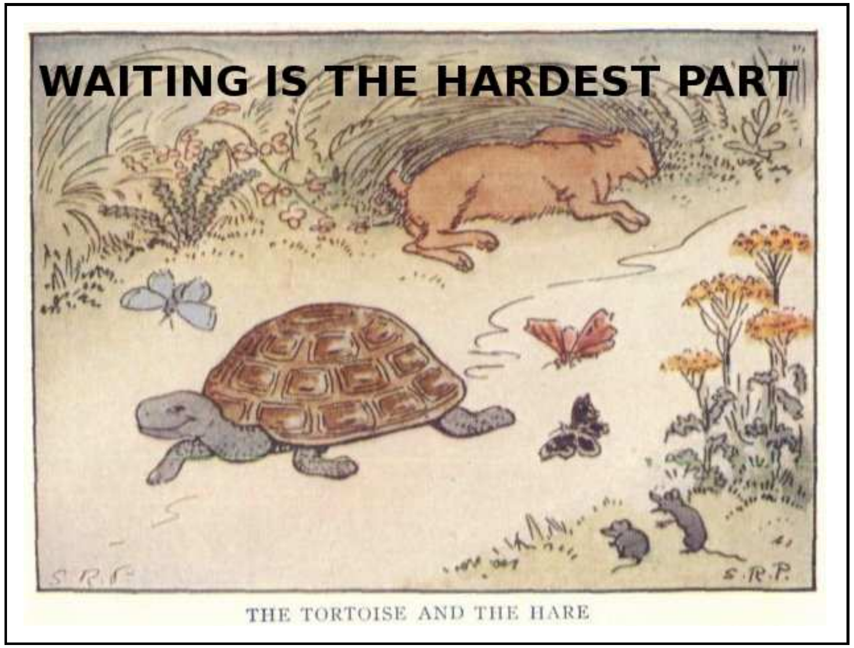


Drawbacks of the TMC method

In TMC:

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

Well, then uncertainty propagation with TMC takes 1000× longer than a single calculation...
(*Each* $\sigma_{\text{statistics}}$ *needs to be small*)



There is a solution with Monte Carlo codes.

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.

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

run 0	ENDF/B-VII.1	seed s_0	*m* histories	T sec.	$k \pm \sigma_{stat}$

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.

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

run 0	ENDF/B-VII.1	seed s_0	m histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s_1	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat}\sqrt{n}$

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.

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

run 0	ENDF/B-VII.1	seed s_0	m histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s_1	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat}\sqrt{n}$
run 2	nuclear data 2	seed s_2	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$

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

run 0	ENDF/B-VII.1	seed s_0	m histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s_1	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat}\sqrt{n}$
run 2	nuclear data 2	seed s_2	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
$\vdots$		$\vdots$			$\vdots$
run n	nuclear data n	seed s_n	m/n hist.	T/n sec.	$k_n \pm \sigma_n$

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

run 0	ENDF/B-VII.1	seed s_0	m histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s_1	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat}\sqrt{n}$
run 2	nuclear data 2	seed s_2	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
⋮		⋮			⋮
run n	nuclear data n	seed s_n	m/n hist.	T/n sec.	$k_n \pm \sigma_n$
n runs				T sec.	

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

run 0	ENDF/B-VII.1	seed s_0	m histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s_1	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat}\sqrt{n}$
run 2	nuclear data 2	seed s_2	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
⋮		⋮			⋮
run n	nuclear data n	seed s_n	m/n hist.	T/n sec.	$k_n \pm \sigma_n$
n runs				T sec.	

$$\left\{ \sigma^2_{total} = \frac{1}{n-1}\sum_{i=1}^{n}\left(k_i - \bar{k}\right)^2 \right.$$

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

run 0	ENDF/B-VII.1	seed s_0	m histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s_1	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat}\sqrt{n}$
run 2	nuclear data 2	seed s_2	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
$\vdots$		$\vdots$			$\vdots$
run n	nuclear data n	seed s_n	m/n hist.	T/n sec.	$k_n \pm \sigma_n$
n runs				T sec.	

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

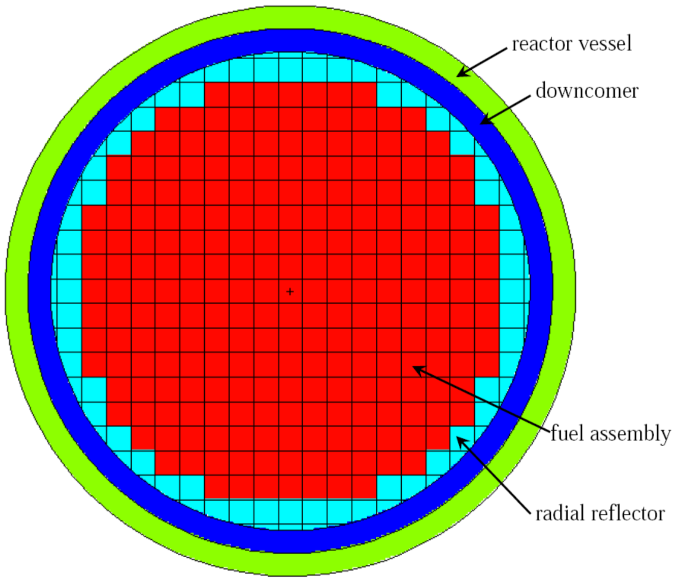
The fast TMC method

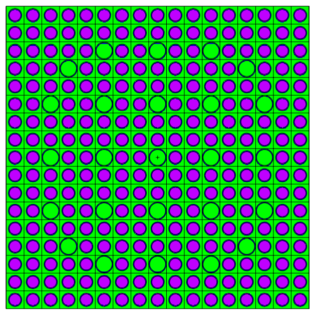
- ☺ as fast as S/U methods (1-2 $\times$ longer than 1 single calculation *without* uncertainties),
- ☺ tested on criticality & shielding benchmarks, burn-up (k_{eff} and inventory),

The fast TMC method

- ☺ as fast as S/U methods (1-2 × longer than 1 single calculation *without* uncertainties),
- ☺ tested on criticality & shielding benchmarks, burn-up (k_{eff} and inventory),
- ☺ Example: the Martin-Hoogenboom benchmark (= the Kord Smith Challenge)

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



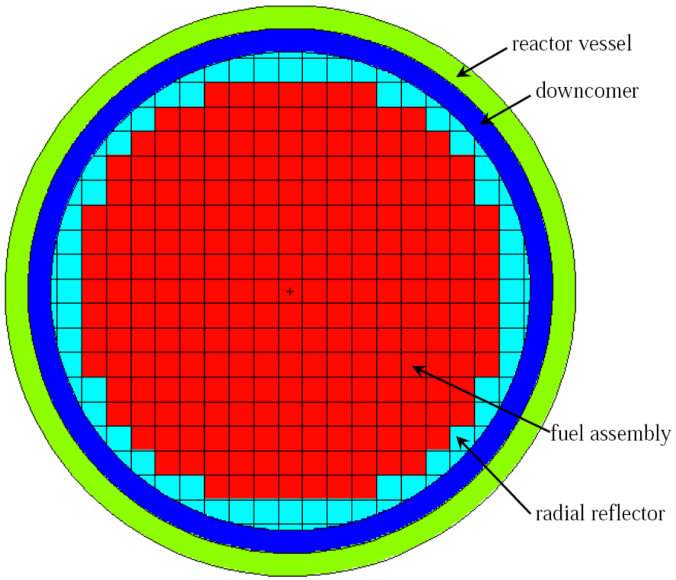


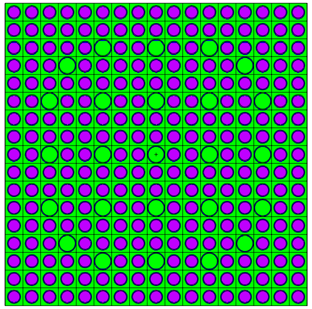
$\Longrightarrow$ 357 × 357 × 100 regions (1.26 × 1.26 × 3.66 cm^3): 12.7 million cells

The fast TMC method

- ☺ as fast as S/U methods (1-2 × longer than 1 single calculation *without* uncertainties),
- ☺ tested on criticality & shielding benchmarks, burn-up (k_{eff} and inventory),
- ☺ Example: the Martin-Hoogenboom benchmark (= the Kord Smith Challenge)

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





$\Longrightarrow$ 357 × 357 × 100 regions (1.26 × 1.26 × 3.66 cm^3): 12.7 million cells

Uncertainty on generated local pin power (tally f7) due to ^{235}U, ^{238}U, ^{239}Pu and H in H_2O thermal scattering in each cell ?

Fast TMC method

1 normal calculation without nuclear data uncertainty takes $n = 2 \times 10^{11}$ histories ($\sigma_{\text{statistics}} = 0.25$ % at the center, 500 weeks on 1 cpu)

$\Longrightarrow$ TMC: 500 random runs of $n = 2 \times 10^{11}$ histories (500 weeks for each)

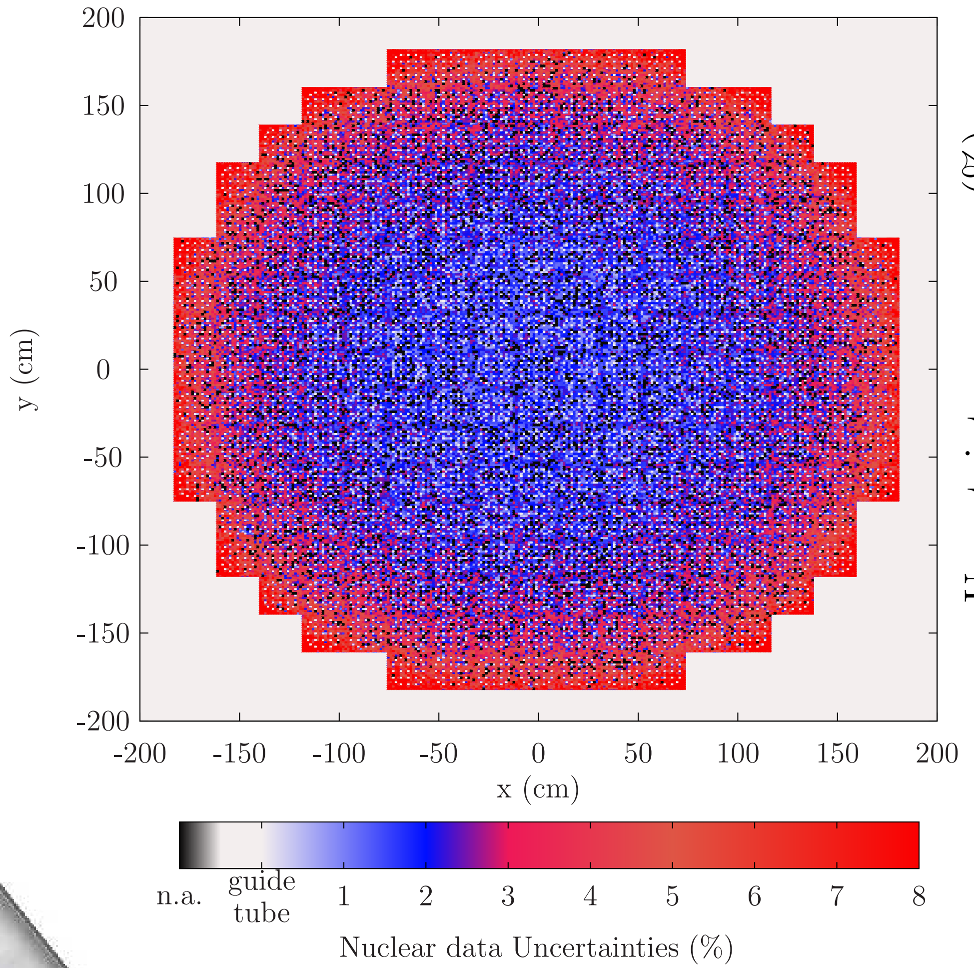
$\Longrightarrow$ fast TMC: 500 random runs of $n/500 = 4 \times 10^{8}$ histories (1 week for each)

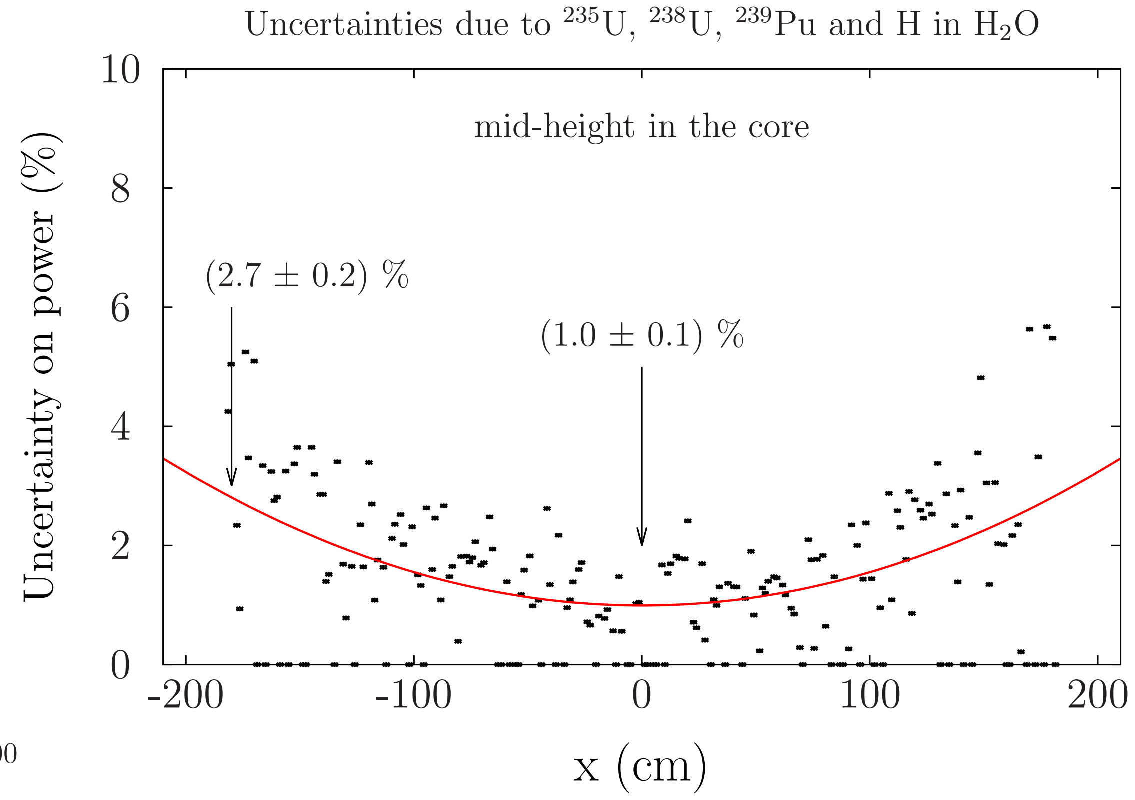
Fast TMC method

1 normal calculation without nuclear data uncertainty takes $n = 2 \times 10^{11}$ histories ($\sigma_{statistics} = 0.25$ % at the center, 500 weeks on 1 cpu)

$\Longrightarrow$ TMC: 500 random runs of $n = 2 \times 10^{11}$ histories (500 weeks for each)

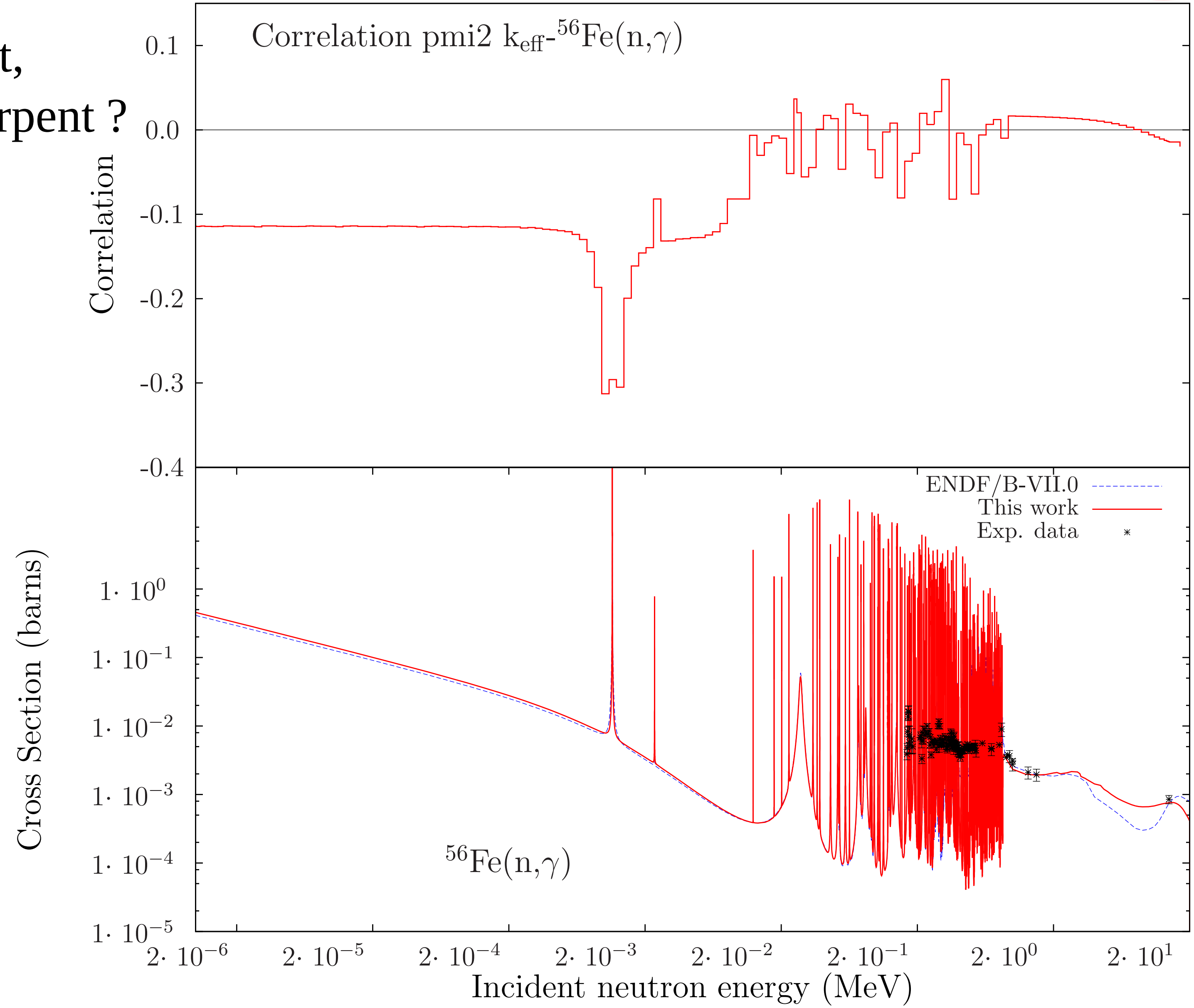
$\Longrightarrow$ fast TMC: 500 random runs of $n/500 = 4 \times 10^{8}$ histories (1 week for each)





Other outcomes of the NRG approach (not detailed here)

- Sensitivity,
- Nuclear data adjustment,
- Include fast TMC in Serpent ?



Conclusions

- (fast) TMC is a powerful tool for uncertainty propagation,
- All types of nuclear data impact can be assessed,
- Most direct way to propagate uncertainties,
- Better QA, better modern use of computers,
- (fast) TMC is part of global approach to improve transparency and safety of nuclear simulation

Conclusions

- (fast) TMC is a powerful tool for uncertainty propagation,
- All types of nuclear data impact can be assessed,
- Most direct way to propagate uncertainties,
- Better QA, better modern use of computers,
- (fast) TMC is part of global approach to improve transparency and safety of nuclear simulation

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

Conclusions

- (fast) TMC is a powerful tool for uncertainty propagation,
- All types of nuclear data impact can be assessed,
- Most direct way to propagate uncertainties,
- Better QA, better modern use of computers,
- (fast) TMC is part of global approach to improve transparency and safety of nuclear simulation

TMC: If we can do a calculation once, we can also do

fast TMC:

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