

# **"Fast Total Monte Carlo" applied to Phase II-2: PWR assembly depletion**

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UAM-7 workshop, Paris, France, April 2013

#### Overview

- ➡ Method: Fast Total Monte Carlo
- Description of the SERPENT model (assembly)
- Considered data in fast TMC

Results



The preliminary report can be found at

ftp://ftp.nrg.eu/pub/www/talys/bib\_rochman/uam-phase2.pdf



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.

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



- $\mathbf{R}$  computer time (not human time),
- Successfully applied (criticality, shielding, reactor, burn-up...)
- Most simple path (no additional processing, no covariance required),
- Many spin-offs (TENDL covariances, sensitivity, adjustment...)
- also applicable to fission yields, thermal scattering, pseudo-fission products, all isotopes (...just everything),



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Well, then uncertainty propagation with TMC takes  $1000 \times \text{longer}$  than a single calculation... (*Each*  $\sigma_{\text{statistics}}$  *needs to be small*) There is at least one solution with Monte Carlo codes: the fast TMC method

#### New method: fast TMC

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

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



New m	New method: fast TMC										
If a	single calcula then reprandon $\sigma_{total}^2 =$	ation tal peat it <i>n</i> n nuclea $\sigma_{\text{statistic}}^2$	kes <i>m</i> histo times with ar data and $+\sigma_{nuclear}^{2}$	pries ( $\sigma_{st}$ h $m/n$ hi random r data still	tat small enough), istories, seeds. holds.						
run 0	ENDF/B-VII.1	seed s <sub>0</sub>	<i>m</i> histories	T sec.	$k\pm\sigma_{stat}$						
run 1	nuclear data 1	seed s <sub>1</sub>	<i>m/n</i> hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat} \sqrt{n}$						

New mo	ethod: fast TMC				No C
If a	single calculation then represented by $\sigma_{total}^2 =$	ation tal peat it <i>n</i> n nuclea $\sigma_{\text{statistic}}^2$	$\frac{1}{2} \cos \frac{m}{2} + \frac{1}{2} \cos \frac{1}$	pries ( $\sigma_{sta}$ n $m/n$ his random r data still	at small enough), stories, seeds. holds.
run 0	ENDF/B-VII.1	seed s <sub>0</sub>	<i>m</i> histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s <sub>1</sub>	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{\text{stat}} \sqrt{n}$
run 2	nuclear data 2	seed s <sub>2</sub>	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$

New mo	ethod: fast TMC	C			
If a	single calcula then reprandom $\sigma_{total}^2 =$	ation tal peat it <i>n</i> n nuclea $\sigma_{\text{statistic}}^2$	kes <i>m</i> histo times with ar data and $c_s + \sigma_{nuclear}^2$	pries ( $\sigma_{sta}$ n $m/n$ his random r data still	t small enough), stories, seeds. holds.
run 0	ENDF/B-VII.1	seed s <sub>0</sub>	<i>m</i> histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s <sub>1</sub>	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{\text{stat}} \sqrt{n}$
run 2	nuclear data 2	seed s <sub>2</sub>	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
• •		• •			• • •
run n	nuclear data <i>n</i>	seed $s_n$	m/n hist.	T/n sec.	$\mathbf{k}_n \pm \mathbf{\sigma}_n$

New me	ethod: fast TMC	2			
If a	single calculation then reprint random $\sigma_{total}^2 =$	ation tal peat it <i>n</i> n nuclea $\sigma^2_{\text{statistic}}$	kes <i>m</i> histo times with ar data and $c_s + \sigma_{nuclea}^2$	pries ( $\sigma_{stat}$ sm h $m/n$ histori random seed r data still hold	nall enough), es, is. ds.
run 0	ENDF/B-VII.1	seed s <sub>0</sub>	<i>m</i> histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s <sub>1</sub>	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat} \sqrt{n}$
run 2	nuclear data 2	seed s <sub>2</sub>	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
• •		•			• • •
run n	nuclear data <i>n</i>	seed $s_n$	m/n hist.	T/n sec.	$\mathbf{k}_n \pm \mathbf{\sigma}_n$
n runs				T sec.	

New mo	ethod: fast TM	С			Nac
If a	single calculation then represented by $\sigma_{total}^2 =$	ation tal peat it <i>n</i> n nuclea $\sigma^2_{\text{statistic}}$	kes <i>m</i> histo times with ar data and $c_s + \sigma_{nuclea}^2$	pries ( $\sigma_{sta}$ h $m/n$ his random r data still	t small enough), stories, seeds. holds.
run 0	ENDF/B-VII.1	seed s <sub>0</sub>	<i>m</i> histories	T sec.	$k \pm \sigma_{stat}$
run 1	nuclear data 1	seed s <sub>1</sub>	m/n hist.	T/n sec.	$k_1 \pm \sigma_1 \sim \sigma_{stat} \sqrt{n}$
run 2	nuclear data 2	seed s <sub>2</sub>	m/n hist.	T/n sec.	$k_2 \pm \sigma_2$
• •		•			• •
run <i>n</i>	nuclear data <i>n</i>	seed $s_n$	m/n hist.	T/n sec.	$\mathbf{k}_n \pm \mathbf{\sigma}_n$
n runs				T sec.	
		$\left\{ \begin{array}{c} \sigma_{total}^2 \\ \end{array} \right.$	$=\frac{1}{n-1}\sum_{i=1}^{n}$	$\sum_{i=1}^{n} \left( k_i - \overline{k} \right)^2 \bigstar$	
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New me	ethod: fast TM	С			Nipo
If a	single calculation then reprint random $\sigma^2$ is the second secon	ation tal peat it <i>n</i> n nuclea $\sigma^2$	$\cos m$ histo times with ar data and $+\sigma^2$	pries ( $\sigma_{sta}$ h $m/n$ his random	at small enough), stories, seeds. holds.
		statistic	s ' nuclear	r data	
	ENDF/B-VII.1	seed s <sub>0</sub>	<i>m</i> mistories	$\frac{1 \text{ sec.}}{T/n \cos 2}$	$\frac{\mathbf{K} \pm \mathbf{O}_{\text{stat}}}{\mathbf{k} \pm \mathbf{\sigma}_{\text{stat}}}$
	nuclear data 1	seed s <sub>1</sub>	m/n mist.		$K_1 \pm O_1 \sim O_{\text{stat}} \sqrt{n}$
run 2	nuclear data 2	seed s <sub>2</sub>	m/n mist.	1/n sec.	$K_2 \pm O_2$
• •		• •			
run <i>n</i>	nuclear data <i>n</i>	seed $s_n$	m/n hist.	T/n sec.	$\mathbf{k}_n \pm \mathbf{\sigma}_n$
n runs		$\begin{cases} \sigma_{total}^{2} \\ \sigma_{statistic}^{2} \end{cases}$	$= \frac{1}{n-1} \sum_{i=1}^{n} \sum_{i=1}^{n} \sigma$	T sec. $\int_{1}^{2} (k_i - \overline{k})^2 \checkmark$	
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### **Description of the SERPENT model (assembly)**

The fuel test is a typical fuel rod from TMI-1 PWR, 15x15 assembly design, see complete description in K. Ivanov (March 2013).



Figure 19: TMI-1 FA Pin Layout

#### Table 47: TMI-1 FA Pin Descriptions

Marker	Rod Type
g	2.0 w/o Gd 4.12% 235U pin
G	Guide Tube
I	Instrumentation Tube
-	4.12% 235U fuel pin



Several hundreds of random ENDF files for transport + depletion

- 3 Major actinides: <sup>235</sup>U, <sup>238</sup>U, <sup>239</sup>Pu,
- 1 Thermal scattering data: H in H<sub>2</sub>O,
- 12 Fission yields: <sup>234,235,236,238</sup>U, <sup>239,240,241</sup>Pu, <sup>237</sup>Np, <sup>241,243</sup>Am, <sup>243,244</sup>Cm,
- 13 Minor actinides: <sup>234,236,237</sup>U, <sup>237</sup>Np, <sup>238,240,241,242</sup>Pu, <sup>241,242g,243</sup>Am, <sup>242,245</sup>Cm
- 138 fission products:  $^{72-74,76}$ Ge,  $^{75}$ As,  $^{76-80,82}$ Se,  $^{79,81}$ Br,  $^{80-84,86}$ Kr,  $^{85,87}$ Rb,  $^{86-88,92}$ Sr,  $^{89}$ Y,  $^{93,95}$ Zr,  $^{94,95}$ Nb,  $^{95-97}$ Mo,  $^{99}$ Tc,  $^{99-104,106}$ Ru,  $^{103,105,106}$ Rh,  $^{104-108,110}$ Pd,  $^{109}$ Ag,  $^{111-114,116}$ Cd,  $^{113,115}$ In,  $^{115,117-119,126}$ Sn,  $^{121,123,125}$ Sb,  $^{122-128,130}$ Te,  $^{127,129,135}$ I,  $^{128,130-132,134-136}$ Xe,  $^{133-137}$ Cs,  $^{134-138}$ Ba,  $^{140}$ La,  $^{140,142}$ Ce,  $^{141,144}$ Pr,  $^{142-146,148,150}$ Nd,  $^{147-149}$ Pm,  $^{147,149-152,154}$ Sm,  $^{151-156}$ Eu,  $^{152,154-158,160}$ Gd,  $^{159,160}$ Tb,  $^{160-164}$ Dy,  $^{165}$ Ho,  $^{166,167}$ Er.

Calculated quantities:  $k_{\infty}$ , rr, macroscopic cross sections (2 groups), ADF, Number densities, relative power pin distribution

# Results on $k_{\infty}$

esults on $k_{\infty}$						- N	RG
		Bu	ırn-up (GWd	/MTU)			
	0	0.2	10	20	30	40	
k <sub>∞</sub>	1.39	1.35	1.26	1.17	1.09	1.02	
Order							
1.	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U	<sup>235</sup> U	<sup>239</sup> Pu	
2.	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U	<sup>235</sup> U	<sup>238</sup> U	<sup>235</sup> U	
3.	H in H <sub>2</sub> O	<sup>239</sup> Pu	<sup>238</sup> U				
	Uno	certainties (in	n %) coming	from			
<sup>235</sup> U	0.56	0.53	0.44	0.40	0.37	0.34	
<sup>238</sup> U	0.41	0.42	0.42	0.42	0.35	0.31	
<sup>239</sup> Pu	-	-	0.15	0.25	0.32	0.38	
H in H <sub>2</sub> O	0.14	0.12	0.24	0.30	0.30	0.28	
Minor Act.	-	-	0.03	0.03	0.06	0.07	
Fiss. Yiel.	-	0.11	0.17	0.22	0.26	0.31	
Lumped F.P.	-	0.05	0.07	0.10	0.14	0.14	
Total	0.71	0.70	0.70	0.74	0.74	0.75	

#### **Results on reaction rates**

s on reac	tion rates	8					-
		Burn-	up (GWd/MT	U) (main contri	ibutor)		
	0	0.2	10	20	30	40	
$^{235}$ U(n, $\gamma$ )	<sup>235</sup> U						
$^{238}$ U(n, $\gamma$ )	<sup>238</sup> U	238	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U	
$^{239}$ Pu(n, $\gamma$ )	H in H <sub>2</sub> O	<sup>239</sup> Pu					
$^{240}$ Pu(n, $\gamma$ )	H in H <sub>2</sub> O						
$^{241}$ Pu(n, $\gamma$ )	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	Minor Act.	<sup>238</sup> U	<sup>238</sup> U	
$^{235}$ U(n,f)	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U	
$^{238}$ U(n,f)	<sup>235</sup> U						
<sup>239</sup> Pu(n,f)	H in H <sub>2</sub> O	<sup>239</sup> Pu	<sup>239</sup> Pu				
$^{240}$ Pu(n,f)	<sup>235</sup> U						
$^{241}$ Pu(n,f)	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U	<sup>238</sup> U	
	Total uncerta	inties (due to	transport data	and fission yie	lds, in %) for		
$^{235}U_{n.\gamma}$	2.06	2.04	2.03	2.14	2.30	2.56	
$^{238}\mathrm{U}_{n,\gamma}$	1.82	1.81	1.72	1.70	1.49	1.31	
$^{239}$ Pu <sub>n,y</sub>	2.68	2.64	2.13	1.96	1.95	2.04	
$^{240}$ Pu <sub>n, Y</sub>	4.89	5.11	4.93	4.55	4.54	4.66	
$^{241}$ Pu <sub><i>n</i>,<math>\gamma</math></sub>	1.80	2.07	1.70	1.67	1.85	2.13	
$^{235}U_{n,f}$	0.57	0.59	0.79	1.17	1.58	2.10	
$^{238}$ U <sub><i>n</i>,<i>f</i></sub>	7.38	7.41	5.78	4.94	4.41	4.10	
$^{239}$ Pu <sub>n,f</sub>	2.24	2.21	2.22	2.12	2.17	2.36	
$^{240}$ Pu <sub>n,f</sub>	3.08	3.11	2.53	2.20	2.02	1.81	
$^{241}$ Pu <sub>n,f</sub>	1.60	1.59	1.32	1.33	1.56	1.93	

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## **Results on macroscopic cross sections**

Results or	ts on macroscopic cross sections										
		Burn-up (GWd/MTU) (main contributor)									
	0	0.2	10	20	30	40					
$\Sigma_{abs1}$	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U					
$\Sigma_{abs2}$	H in $H_2O$	H in H <sub>2</sub> O	H in H <sub>2</sub> O	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U					
$\Sigma_{\rm fiss1}$	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U					
$\Sigma_{\rm fiss2}$	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U					
$\nu \Sigma_{\rm fiss1}$	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U					
$\nu \Sigma_{\rm fiss2}$	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U					
D <sub>iff1</sub>	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U					
D <sub>iff2</sub>	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O					
$\Sigma_{trn1}$	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U					
$\Sigma_{trn2}$	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O					
InvVel <sub>1</sub>	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O					
InvVel <sub>2</sub>	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O					

### **Results on number densities for actinides**

ults on number densities for actinides											
						<b>r</b>	<b>IRG</b>				
	Burn-up (GWd/MTU) (main contributor)										
	0	0.2	10	20	30	40					
<sup>234</sup> U	-	Minor Act.									
<sup>235</sup> U	-	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	235	<sup>238</sup> U					
<sup>236</sup> U	-	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	235	<sup>235</sup> U					
<sup>238</sup> U	-	-	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U	<sup>238</sup> U					
<sup>237</sup> Np	-	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	235	<sup>238</sup> U					
<sup>238</sup> Pu	-	<sup>235</sup> U	<sup>235</sup> U	<sup>235</sup> U	Minor Act.	Minor Act.					
<sup>239</sup> Pu	_	<sup>238</sup> U									
<sup>240</sup> Pu	-	Minor Act.	<sup>238</sup> U	<sup>238</sup> U	H in $H_2O$	H in H <sub>2</sub> O					
<sup>241</sup> Pu	_	H in H <sub>2</sub> O									
<sup>242</sup> Pu	-	H in H <sub>2</sub> O									
<sup>241</sup> Am	_	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	Minor Act.	Minor Act.					
<sup>243</sup> Am	_	H in H <sub>2</sub> O									
<sup>242</sup> Cm	-	H in H <sub>2</sub> O	H in H <sub>2</sub> O	H in H <sub>2</sub> O	Minor Act.	Minor Act.					
<sup>244</sup> Cm	-	H in H <sub>2</sub> O									

### **Results on number densities for fission products**

- N	RG

	Burn-up (GWd/MTU) (main contributor)					
	0	0.2	10	20	30	40
<sup>90</sup> Sr	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>95</sup> Mo	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>99</sup> Tc	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
$^{101}$ Ru	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>103</sup> Rh	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>109</sup> Ag	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>129</sup> I	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>133</sup> Xe	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>135</sup> Xe	-	Minor Act.	Minor Act.	Minor Act.	Minor Act.	Minor Act.
<sup>133</sup> Cs	_	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
$^{134}Cs$	_	Minor Act.	Minor Act.	Minor Act.	Minor Act.	Minor Act.
<sup>137</sup> Cs	_	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>144</sup> Ce	_	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>142</sup> Nd	_	Minor Act.	Minor Act.	Minor Act.	Minor Act.	Minor Act.
<sup>143–148</sup> Nd	_	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
$^{147-152}$ Sm	-	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>153–155</sup> Eu	_	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
<sup>155–158</sup> Gd	_	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields	Fiss. Yields
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#### Example for $k_\infty$



#### Comparison of $\Delta k_\infty$



#### Local power density

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The pin power distribution and burnup of each fuel pin (in GWd/t) as well as the associated uncertainties is requested with one unique material definition for all pins. Is that the best ? We varied all nuclear data separately  $\implies$  no visible effect

Better to vary all of them together (to be done).

#### Conclusions



- fast TMC successfully applied for this PWR assembly benchmark,
- Transport nuclear data, fission yields and thermal scattering were considered,
- Importance of  $^{235,238}$ U,  $^{239}$ Pu and thermal scattering (H in H<sub>2</sub>O),
- $\checkmark$  (and fission yields for number densities),
- ➡ Minor actinides and fission products are of less importance.

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