Assessment of the MCNP-ACAB code system for burnup credit analyses

N. García-Herranz, O. Cabellos, J. Sanz

UPM - UNED

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- Uncertainty propagation by a hybrid Monte Carlo method

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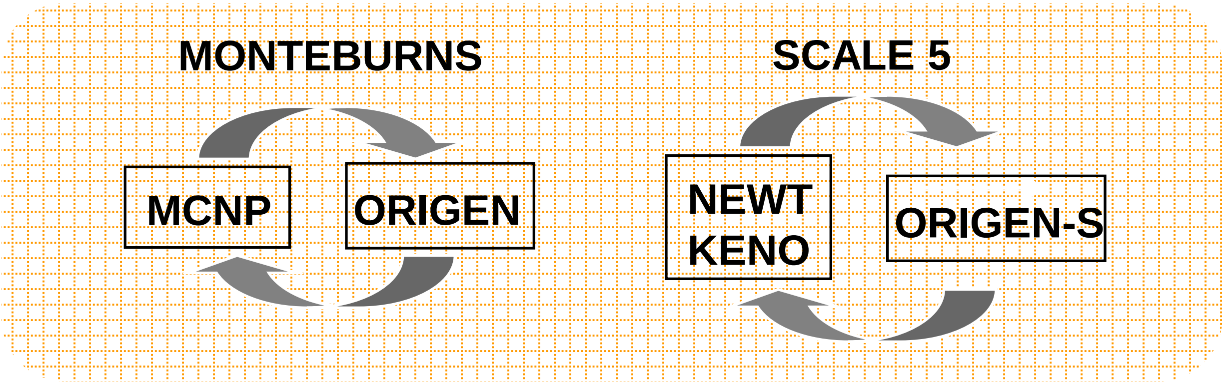
Introduction

- Burn-up credit analyses are based on depletion calculations that provide an accurate prediction of spent fuel isotopic contents, followed by criticality calculations to assess k_{eff}

- Different systems coupling a neutron transport code with an isotopic inventory code are being applied:



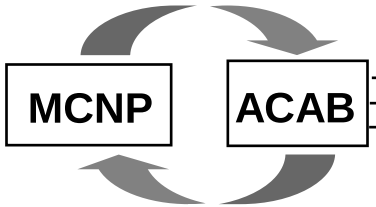
- In order to have confidence in the results $\rightarrow$ need of evaluating uncertainties in isotopics for spent fuel and assess their potential impact on reactivity
  - uncertainties in the basic data
  - assumptions made in the calculation models

Introduction

- Many efforts in last years focused on investigating the impact of the large variety of reactor operating conditions (fuel T, moderator/density T, burn-up profile, …)

- **Our goal**: to present the capabilities of the MCNP-ACAB system, which combines MCNP and the inventory code ACAB, as a suitable tool for burn-up credit calculations

- **By means of ACAB capabilities**, the system allows computing:



Isotopic inventory dealing with all nuclear processes that can occur in a high-burnup fuel regime

Isotopic-related quantities useful for safety and waste management assesment (decay heat, neutron emission, radiotoxicity, ...)

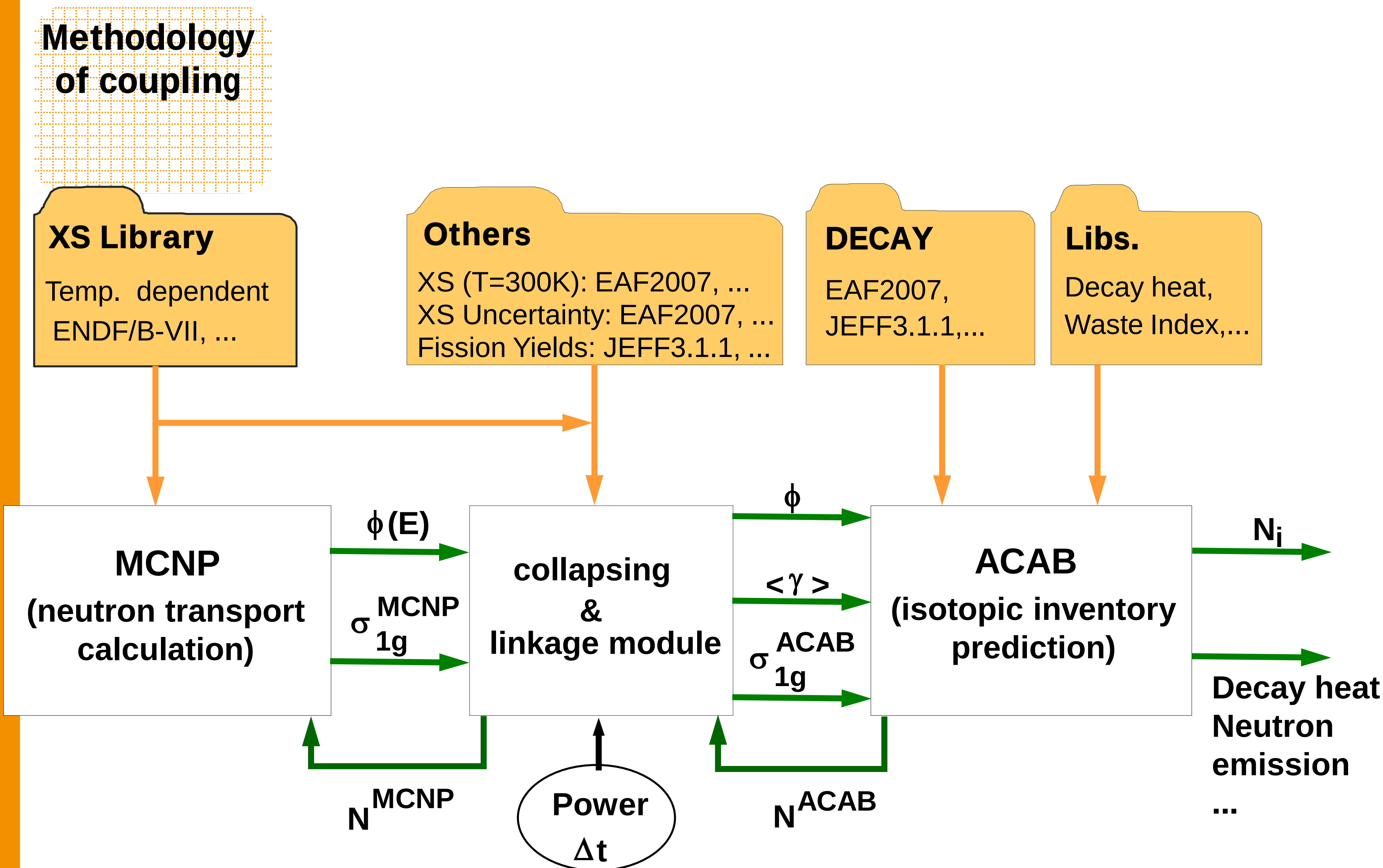
Uncertainties in the prediction of the isotopic inventory as well as in the different inventory-related response functions

MCNP-ACAB code system

ACAB

- Computational algorithm based on that ORIGEN
- Capability of treating the possible decay transitions from ground, first and second isomeric states
- The most updated nuclear data libraries can be easily processed:
  - ✓ Nuclear reaction cross-section data : EAF2007, JEFF-3.1.1,…
  - ✓ Nuclear decay data : EAF2007, …
  - ✓ Fission product yields : JEFF-3.1.1, …
  - ✓ Uncertainty libraries : EAF2007/UN, …
- Uncertainty propagation by two methodologies: sensitivity and Monte Carlo
- Code widely validated against benchmarks, experiments and other depletion codes

MCNP-ACAB code system



Propagation of uncertainties in Monte Carlo burn-up calculations

Sources of uncertainties in a depletion calculation

$$\frac{dN}{dt} = \boldsymbol{A}N = [\lambda]N + \left[\boldsymbol{\sigma}^{eff}\right]\Phi N$$

$$N = N\left(\lambda, \sigma^{eff}, \Phi\right) = N(\lambda, \sigma^{g}, \phi^{g}(E), \Phi)$$

- Uncertainties in decay constants Δ_{λ}
- Uncertainties in one-group effective xs $\Delta_{\sigma^{eff}}$

  $$\sigma^{eff} = \sum_{g} \sigma^{g} \phi^{g} \Big/ \sum_{g} \phi^{g}$$

  uncertainties in the evaluated nuclear xs data $\Delta_{\sigma^{g}}$

  uncertainties in the flux spectrum obtained from the transport calculation $\Delta_{\phi^{g}(E)}$
- Uncertainties in the integrated neutron flux Δ_{Φ}

Propagation of uncertainties in Monte Carlo burn-up calculations

Sources of uncertainties in a depletion calculation

- The influence of all these sources should be investigated in order to understand and quantify the uncertainties associated with computer code predictions for spent fuel isotopics

- So far, we have only investigated the influence of uncertainties in activation cross sections and statistical errors in the neutron flux spectrum

  - ✓ No uncertainties in decay constants, fission yields, …
  - ✓ No uncertainties in the integrated neutron flux
  - ✓ Uncertainties in the transport input data lead to smaller errors in the flux spectrum than the statistical fluctuations

$$N = N\left(\lambda, \sigma^{eff}, \Phi\right) = N(\cancel{\lambda}, \sigma^{g}, \phi^{g}(E), \cancel{\Phi})$$

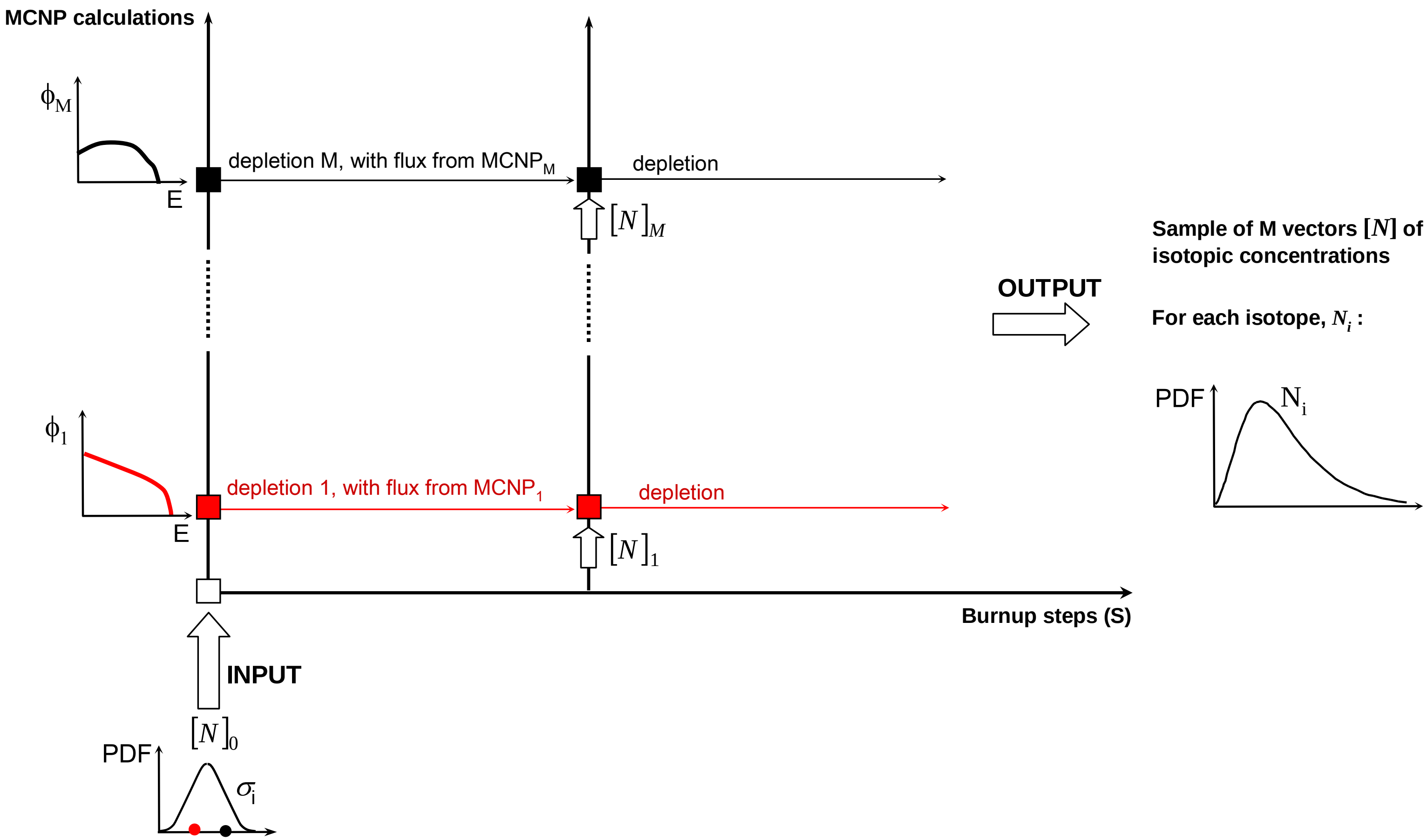
- Useful for burnup credit: e.g. the actual environment conditions during fuel irradiation will produce spectral shifts whose effects in the inventory could be evaluated in a similar way

Propagation of uncertainties in Monte Carlo burn-up calculations

“Brute force” random sampling method

Same sequence followed in the coupled calculation scheme to infer an error propagation procedure throughout the time

Simultaneous random sampling of the PDF of all the input parameters



Propagation of uncertainties in Monte Carlo burn-up calculations

Sensitivity/ Uncertainty Analysis (S/U)

Procedure based on a **first order Taylor** series approach

$$N_i(\sigma^{eff}) = N_i(\hat{\sigma}^{eff}) + \sum_{j=1}^{R}\left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\hat{\sigma}^{eff}}\left(\sigma_j^{eff} - \hat{\sigma}_j^{eff}\right) + \ldots$$

Sensitivity coefficient ρ_{ij}

ε_j error in the 1-G effective xs

$$\sigma_j^{eff} = \sum_g \sigma_j^g \phi^g$$

$$\varepsilon_j = \sum_{g=1}^{G}\phi^g\left(\sigma_j^g - \hat{\sigma}_j^g\right) + \sum_{g=1}^{G}\sigma_j^g\left(\phi^g - \hat{\phi}^g\right) = \phi^T \boxed{\varepsilon_{\sigma_j}} + \sigma_j^T \boxed{\varepsilon_\phi}$$

errors due to uncertainties in the multigroup xs $\left[COV_{\sigma_j}\right]$

to be processed from the uncertainty libraries

errors due to uncertainties in the multigroup flux spectrum $\left[COV_\phi\right]$

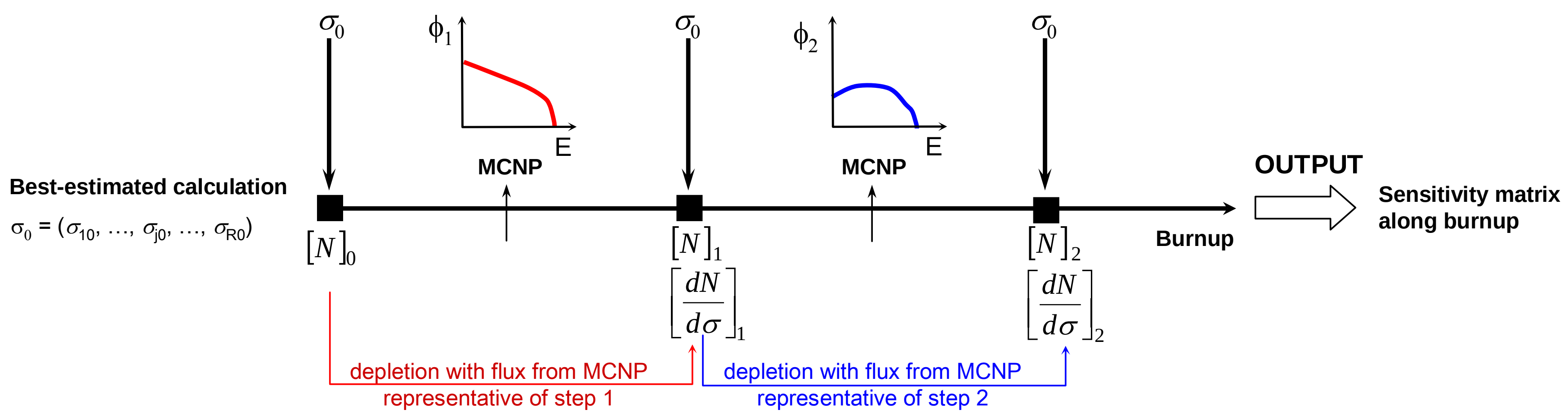
to be obtained from a single MCNP calculation

Propagation of uncertainties in Monte Carlo burn-up calculations

Sensitivity/ Uncertainty Analysis (S/U)

$$N\left(\sigma^{eff}\right) - N\left(\hat{\sigma}^{eff}\right) \approx \boldsymbol{S}\,\varepsilon$$

$$var\,N \approx \boldsymbol{S}\left[COV_{\sigma^{eff}}\right]\boldsymbol{S}^{\boldsymbol{T}} \approx \boldsymbol{S}\left\{ \underbrace{\begin{bmatrix} \ddots & & 0 & \\ 0 & & \hat{\phi}^{T}\left[COV_{\sigma_j}\right]\hat{\phi} & \\ & & & \ddots \end{bmatrix}}_{\text{Propagates the multigroup xs uncertainties when there is no statistical flux errors}} + \underbrace{\begin{bmatrix} \ddots & & 0 & \\ 0 & & \hat{\sigma}_j^{\,T}\left[COV_{\phi}\right]\hat{\sigma}_j & \\ & & & \ddots \end{bmatrix}}_{\text{Propagates statistical flux errors when there is no multigroup xs covariances}} \right\} \boldsymbol{S}^{\boldsymbol{T}}$$



Propagation of uncertainties in Monte Carlo burn-up calculations

Hybrid Monte Carlo method

Based on a **random sampling** $\Rightarrow$ a PDF is assigned to each involved variable

Propagating uncertainties in XS

✓ The PDF is assumed to be lognormal

$$\boxed{\log\left(\frac{\sigma_j^g}{\sigma_{j0}^g}\right) \rightarrow N(0, \Delta_j^g)}$$

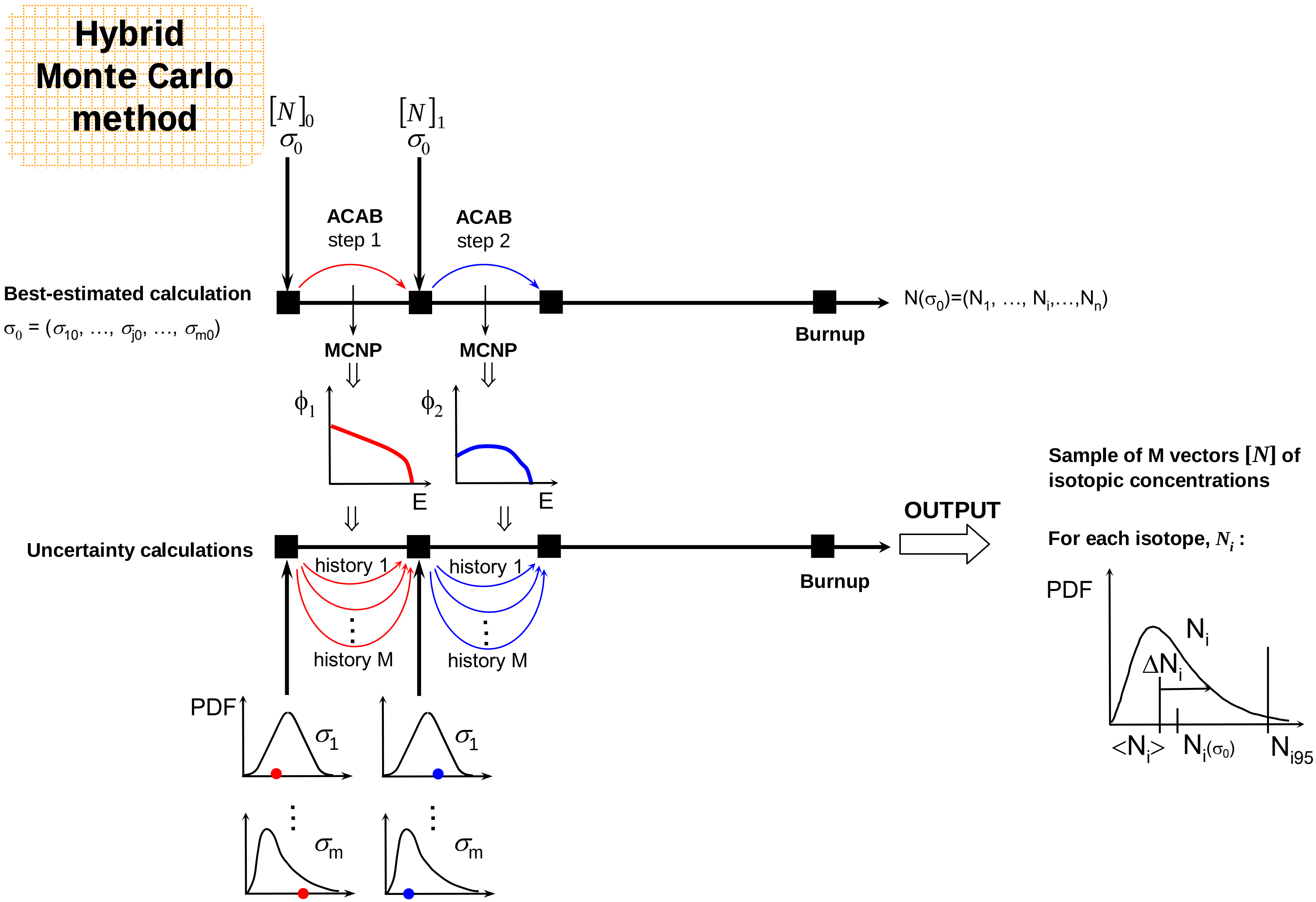
Propagating flux errors

✓ The flux fits a normal distribution

$$\boxed{\phi^g \rightarrow N\left(\hat{\phi}^g, \hat{s}\left(\hat{\phi}_g\right)\right)}$$

We use simultaneous random sampling of all the PDFs involved in the problem to predict the concentration of each nuclide

Propagation of uncertainties in Monte Carlo burn-up calculations

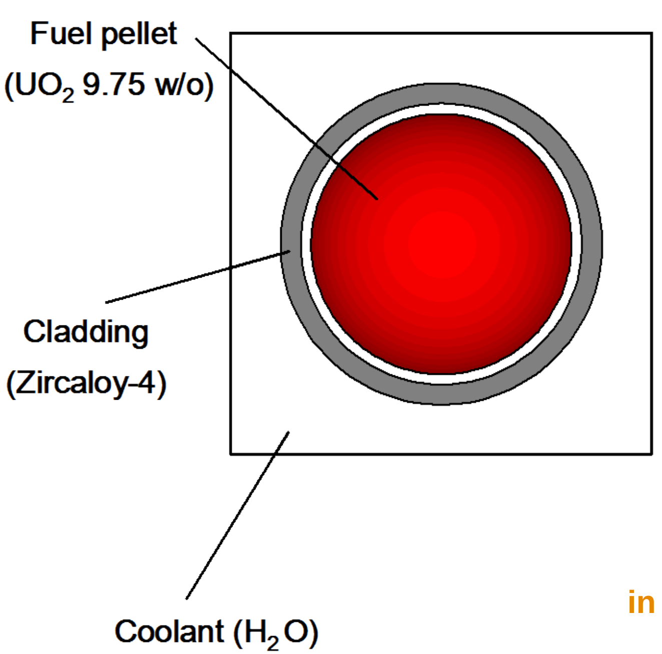


PWR Pin Cell Benchmark

Objective Validate MCNP-ACAB for high-burnup applications

Int. Conf. On Mathematics and Computation, M&C2005

2-D single pin-cell of a standard W 17x17 PWR assembly



	CASMO-4	MCODE	MONTE-BURNS	MCNP-ACAB
	Studsvik	MIT	LANL	UPM
Transport Code	Deterministic	MCNP-4C	MCNP-4C	MCNP-4C
Depletion Code	-	ORIGEN2.1	ORIGEN2.2	ACAB
Coupling algorithm	predictor-corrector	predictor-corrector	middle-timestep	middle-timestep
XS Libraries in transport calculations	ENDF/B-6 JEF-2.2	ENDF/B-5 ENDF/B-6 + other evaluated libraries	ENDF/B-5 ENDF/B-6 JENDL3.2	
Libraries in burnup and decay calculations		PWRUE.LIB DECAY.LIB		

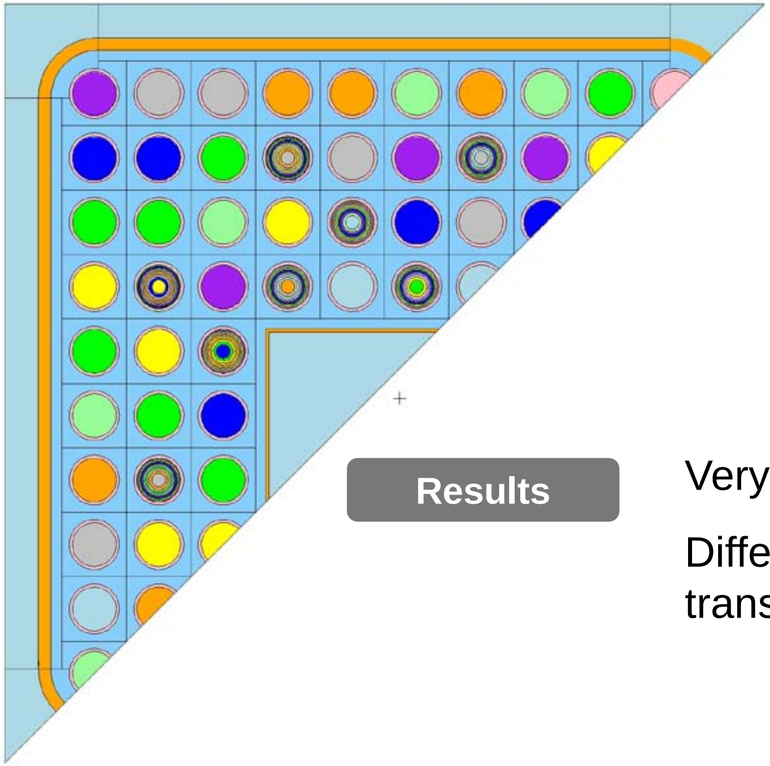
Validation

BWR Atrium-10XP assembly

Objective

Comparison MCNP-ACAB vs MONTEBURNS to predict the isotopics along burnup

Int. Congress on Nuclear Fuel, TOPFUEL2006



- 65 materials
- 60 burnup steps (up to 60 GWd/tU)
- 200 000 histories

Results

Very similar isotopics for most of nuclides.

Differences in some minor actinides due to isomeric transition treatment

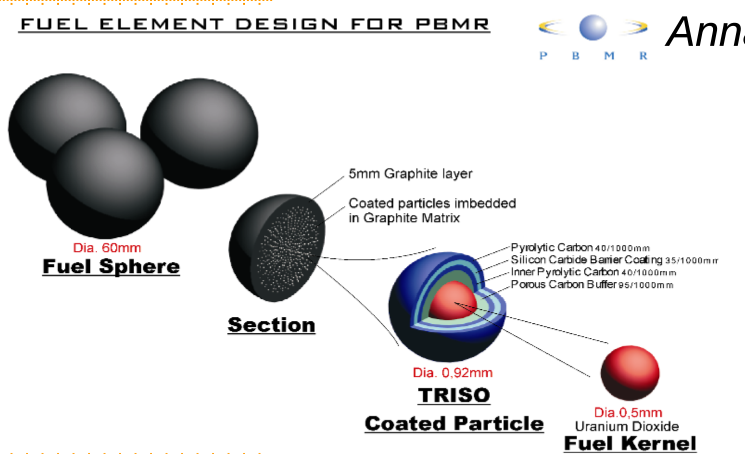
Validation

HTR Plutonium Cell Burnup Benchmark

Objective

Validation of several code systems to be used for the analysis of HTR up to unusually high burn-up of 800 MWd/kgHM – Case “C1” with 1.5 g Pu per fuel element

Annals of Nuclear Energy, 35, 2008



Main requested calculations

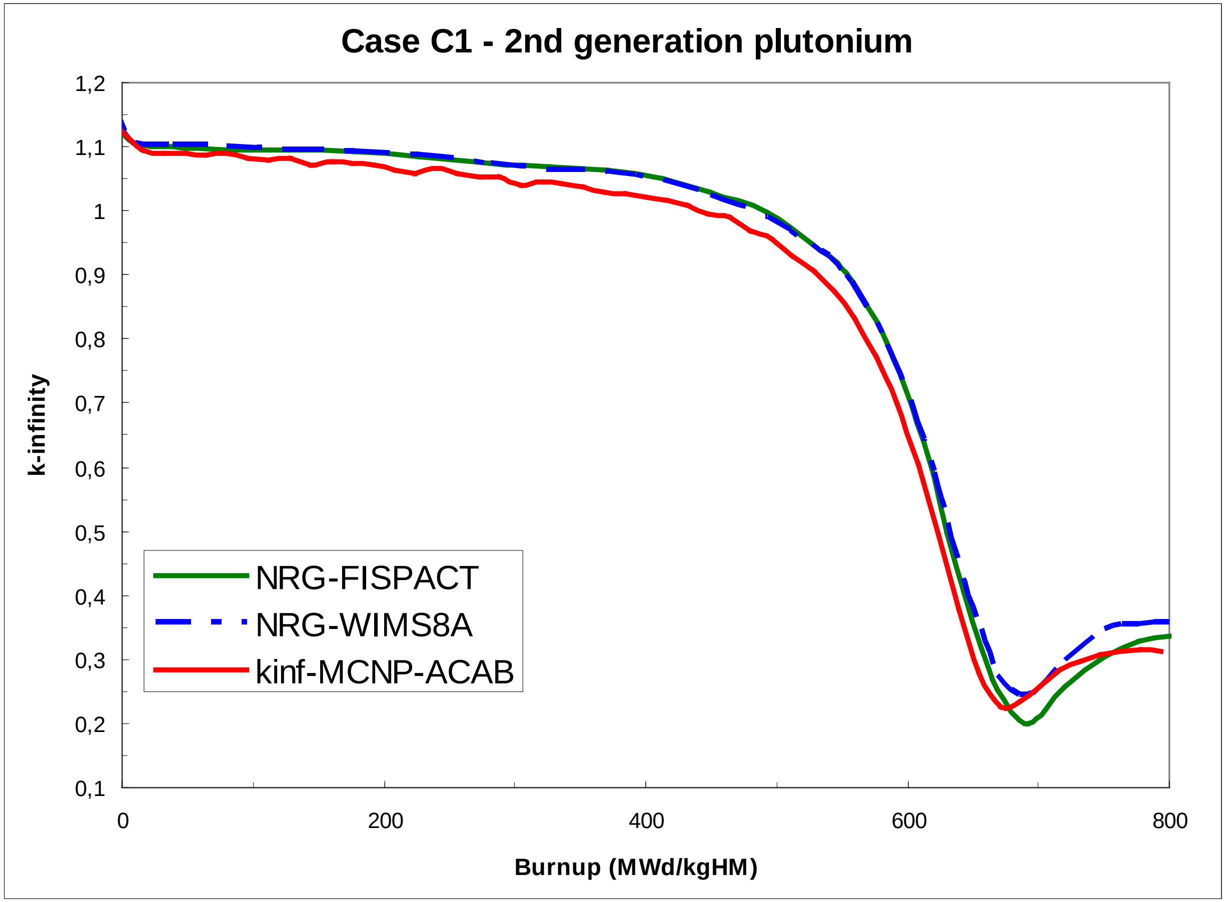
- Multiplication factor
- Isotopic composition during the irradiation
- 1200 full power days
- Comparisons with NRG calculations

	NRG-WIMS	**NRG-OCTOPUS**	**MCNP-ACAB**
Transport code	WIMS8A	MCNP-4C3	MCNP-4C3
Depletion code		FISPACT	ACAB
Coupling algorithm		Predictor step	Middle-time step approach
Burn-up steps	230	230	50
XS libraries	JEFF-2.2 based 172-group	JEFF-2.2 based point energy EAF4 UN library	JEFF-3.1 / EAF2005 / JEFF-2.2 fission yields EAF2005 UN library

Validation

HTR Plutonium Cell Burnup Benchmark

Results with no uncertainties



Validation

HTR Plutonium Cell Burnup Benchmark

Results with no uncertainties

Table 1. Nuclide densities of some Pu isotopes as function of burn-up, taking NRG-WIMS as reference solution. For the other solutions the relative difference respect to WIMS is given

Isotopes	Burn-up (MWd/kgHM)	NRG-WIMS (10^{24} at /cm^3)	NRG-OCTOPUS (%)	MCNP-ACAB (%)
Pu-239	100	4.16E-03	-1.48	-0.24
	400	6.18E-04	-7.41	-1.48
	600	7.39E-05	-2.10	-10.31
	800	6.29E-08	-29.82	-23.09
Pu-240	100	6.66E-03	1.10	1.94
	400	2.87E-03	1.42	7.10
	600	5.77E-04	-0.71	-11.64
	800	2.50E-06	-1.79	14.64
Pu-241	100	4.12E-03	-0.57	-1.36
	400	2.98E-03	-1.97	0.18
	600	4.37E-04	-8.37	-11.91
	800	5.78E-07	-7.38	9.70

Validation

HTR Plutonium Cell Burnup Benchmark

Results with uncertainties: Impact of xs uncertainties

Table 2. Calculated uncertainties in the some Pu concentrations due to cross section uncertainties as function of burn-up

Isotopes	Burn-up (MWd/kgHM)	NRG-OCTOPUS (%)	MCNP-ACAB (%)
Pu-239	100	5.11	3.48
	400	27.04	7.92
	600	16.06	16.58
	800	46.67	23.83
Pu-240	100	3.77	2.88
	400	13.31	5.00
	600	25.82	12.32
	800	15.39	9.89
Pu-241	100	4.21	1.97
	400	9.30	4.13
	600	18.30	23.78
	800	15.10	9.58

Validation

HTR Plutonium Cell Burnup Benchmark

Results with uncertainties: Impact of xs uncertainties and flux errors

- ✓ Different number of histories in MCNP calculations have been considered in order to have different qualities of the transport calculations, that is, flux spectrum relative errors of different order of magnitude

Table 3. Different MCNP calculations to compute the neutron flux spectrum

Number of histories	**Relative error (%) in k-eff**	**Order of magnitude of the relative errors (%) in the flux tallies**
5k (50 cycles with 100 histories/cycle)	1.18	~12
50k (50 cycles with 1k histories/cycle)	0.29	~5
500k (50 cycles with 10k histories/cycle)	0.11	~2

Validation

HTR Plutonium Cell Burnup Benchmark

Results with uncertainties: Impact of xs uncertainties and flux errors

Table 4. Relative error (%) of the final concentration computed by the **Monte Carlo technique**.

Isotope	Only due to XS errors Neutron histories			Only due to flux errors Neutron histories			Total errors Neutron histories		
	500k	50k	5k	500k	50k	5k	500k	50k	5k
Pu 238	19.48	19.56	19.40	0.85	2.72	8.57	19.50	19.77	21.35
Pu 239	15.95	16.46	16.05	0.69	2.19	6.94	15.97	16.63	17.53
Pu 240	20.35	19.60	19.68	0.79	2.45	7.69	20.36	19.74	21.09
Pu 241	19.28	19.14	18.72	0.74	2.20	6.97	19.29	19.26	19.86
Pu 242	46.01	47.50	46.22	1.58	5.00	16.49	46.04	47.79	48.99
Pu 244	7.71	7.20	7.07	0.08	0.26	0.81	7.71	7.20	7.11

Table 5. Relative errors (%) of the final isotopic concentration computed by **sensitivity.**

Isotope	Only due to XS errors Neutron histories			Only due to flux errors Neutron histories			Total errors Neutron histories		
	500k	50k	5k	500k	50k	5k	500k	50k	5k
Pu 238	19.13	19.14	19.03	0.88	2.78	8.62	19.15	19.34	20.90
Pu 239	16.03	16.04	15.95	0.71	2.25	6.95	16.05	16.20	17.40
Pu 240	20.82	20.75	20.53	0.78	2.47	7.80	20.83	20.90	21.96
Pu 241	20.09	20.02	19.79	0.70	2.24	7.07	20.10	20.14	21.02
Pu 242	46.45	46.35	46.08	1.58	5.00	15.79	46.47	46.62	48.71
Pu 244	7.02	7.01	6.95	0.08	0.26	0.84	7.02	7.02	7.00

Conclusions

- ✓ An automated tool called MCNP-ACAB that links MCNP with our inventory code ACAB is presented

- ✓ It has been successfully applied to different benchmarks to predict the isotopic inventory in high-burnup calculations

- ✓ It enables to estimate the impact of neutron cross section uncertainties as well as neutron flux statistical errors on the inventory in transport-burn-up combined problems, by using either a sensitivity/uncertainty or a Monte Carlo propagation technique. Uncertainties in the predicted decay heat, neutron emission, … can be obtained in a similar way

- ✓ Both uncertainty methodologies are acceptable to deal with the benchmark problem. Even at very high burn-ups, such as 800 MWd/kgHM, non-linear effects are not important and the sensitivity method is useful to infer isotopic uncertainties

- ✓ Provided that the flux statistical deviations in the MC transport calculation do not exceed a given value, the effect of the flux errors in the calculated isotopic inventory are negligible compared to the effect of the large xs uncertainties available at present in the data files

Ongoing work

- ✓ Validation of MCNP-ACAB for burnup credit analysis will be performed to quantify biases and uncertainties between analytic predictions and measured isotopics

- ✓ In order to estimate uncertainties, the methodologies already implemented could be useful to achieve a better understanding of the influence of some assumptions made in the depletion calculations

- ✓ For example, it could be useful to evaluate the effects of the spectral shift due to 2D/3D environmental conditions during fuel irradiation

- ✓ The influence of the other sources of uncertainties should also be evaluated and further developments in this area will be needed. This is the case of the effect of the normalization factor (i.e. effect of the power when held constant with time)

Thank you for your attention