Strategies for the uncertainty quantification of fuel cycle scenarios

Aris V. Skarbeli
F. Álvarez-Velarde

CIEMAT

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Contents

Sensitivity analysis

Sensitivity coefficients (local)

$$V(y) \approx \sum_{i=1}^{d} \left(\frac{\partial y}{\partial x_i} \right)^2 V(x_i)$$

- ✗ First order perturbation
- ✗ Lineal and separable variables
- ✓ Fast to compute

Sobol indices (global)

$$V(y) = \sum_{i=1}^{d} V_i + \sum_{i \le i \le j \le d} V_{ij} + \cdots + V_{i,\ldots,d}$$

- ✓ Use all the input parameter space
- ✓ Any kind of dependence
- ✗ High computational demand

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$2d+1$ terms in the expansion $\Longrightarrow$ first and total order coefficients

$$S_i = \frac{V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))}{V(Y)} \qquad ST_i = \frac{E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y|\mathbf{X}_{\sim i}))}{V(Y)}$$

$$\left(\sum S_i \leq 1\,,\;\; ST_i \geq S_i\right)$$

$$V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i)) = \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{X}')_j(f(\mathbf{X}_{\sim i}, X_i')_j - f(\mathbf{X})_j)$$

$$E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y|\mathbf{X}_{\sim i})) = \frac{1}{2N}\sum_{j=1}^{N}(f(\mathbf{X})_j - f(\mathbf{X}_{\sim i}, X_i')_j)^2$$

Integrals up to $2d$ dimensions

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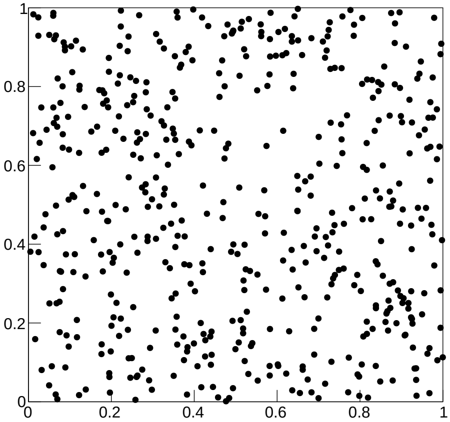
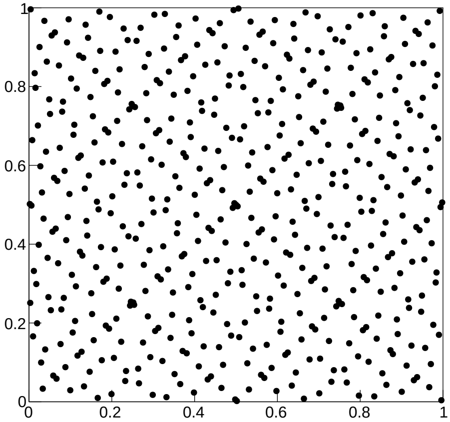
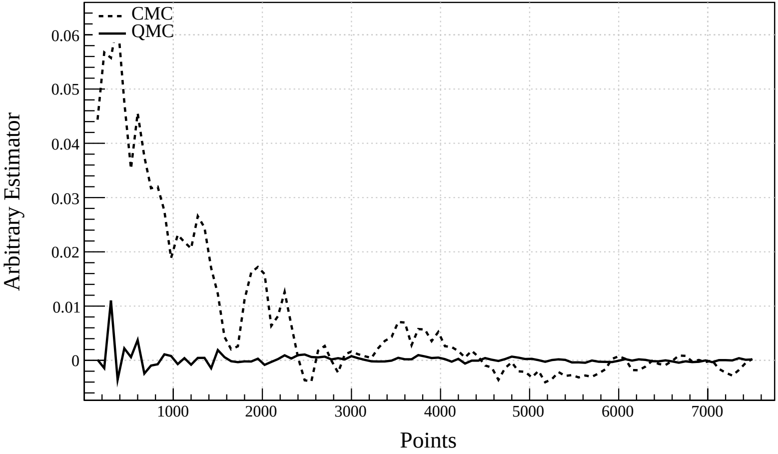
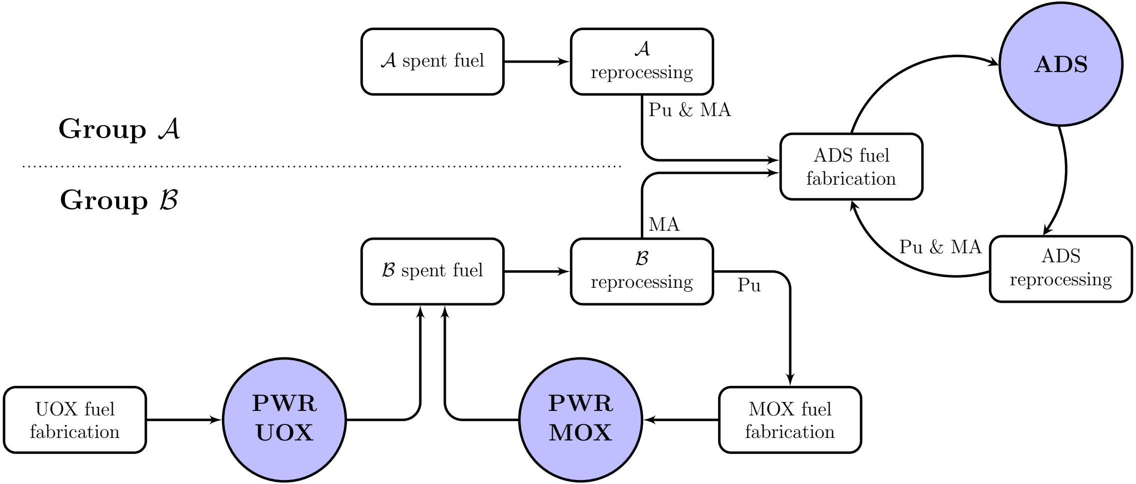
Crude Monte Carlo (CMC) $\mathcal{O}(1/\sqrt{N})$



Sobol sequence (QMC) $\mathcal{O}(\log^d(N)/N)$




CMC
QMC
0.06
0.05
0.04
0.03
0.02
0.01
0
Arbitrary Estimator
1000
2000
3000
4000
5000
6000
7000
Points



$\mathcal{A}$ spent fuel
$\mathcal{A}$ reprocessing
Pu & MA
ADS
Group $\mathcal{A}$
ADS fuel fabrication
Group $\mathcal{B}$
MA
Pu & MA
ADS reprocessing
$\mathcal{B}$ spent fuel
$\mathcal{B}$ reprocessing
Pu
UOX fuel fabrication
PWR UOX
PWR MOX
MOX fuel fabrication

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Parameter	Ref.Value	Units	Parameter	Ref.Value	Units
PWR Park energy	430	TWh_e	ADS burn-up	78.3	GWd/t_{HM}
PWR MOX ratio	10	%	$\mathcal{A}$ UOX SF	100	%
UOX electric power	1000	MW_e	$\mathcal{A}$ MOX SF	100	%
UOX thermal efficiency	33	%	$\mathcal{B}$ UOX SF	100	%
UOX core mass	78.545	t_{HM}	$\mathcal{B}$ MOX SF	100	%
PWR load factor	0.8	—	Repr. capacity UOX	1700.0	t_{HM}/y
UOX burn-up	50.0	GWd/t_{HM}	Repr. capacity MOX	120.0	t_{HM}/y
MOX electric power	1000	MW_e	Repr. capacity $\mathcal{A}$	850.0	t_{HM}/y
MOX thermal efficiency	33	%	Hydrometallurgical sep. eff. Pu	99.9	%
MOX core mass	78.545	—	Hydrometallurgical sep. eff. MA	99.9	%
MOX burn-up	50.0	GWd/t_{HM}	Pyrometallurgical sep. eff. Pu	99.9	%
ADS phase 1 energy	24.66	TWh_e	Pyrometallurgical sep. eff. MA	99.9	%
ADS phase 2 energy	15.27	TWh_e	UOX enrichment	4.2	%
ADS electric power	154	MW_e	Enrichment tails	0.25	%
ADS thermal efficiency	0.40	%	Pu in MOX fuel	8.5	%
ADS core mass	5.325	t_{HM}	Pu in ADS fuel	45	%
ADS load factor	0.87	—			

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EVOLCODE

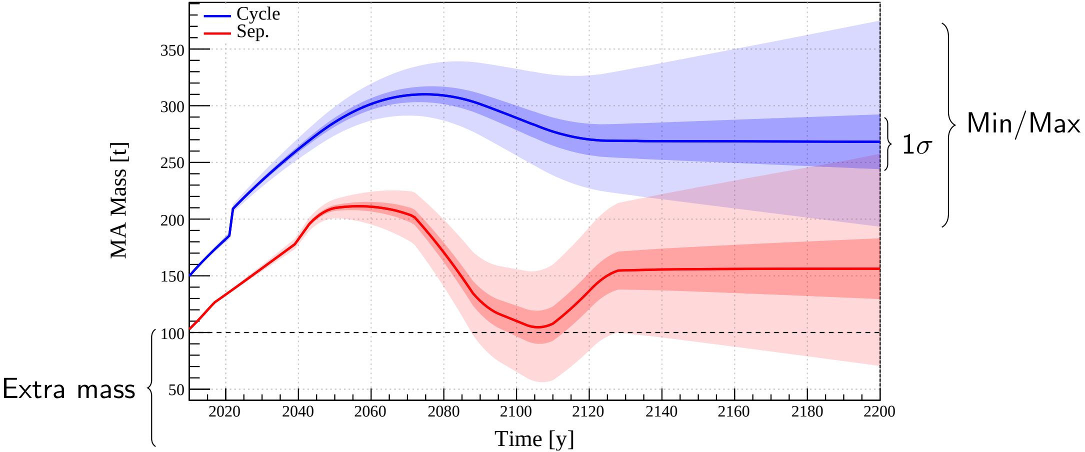
- Coupling between neutronic and depletion codes
- Specific irradiation libraries generation

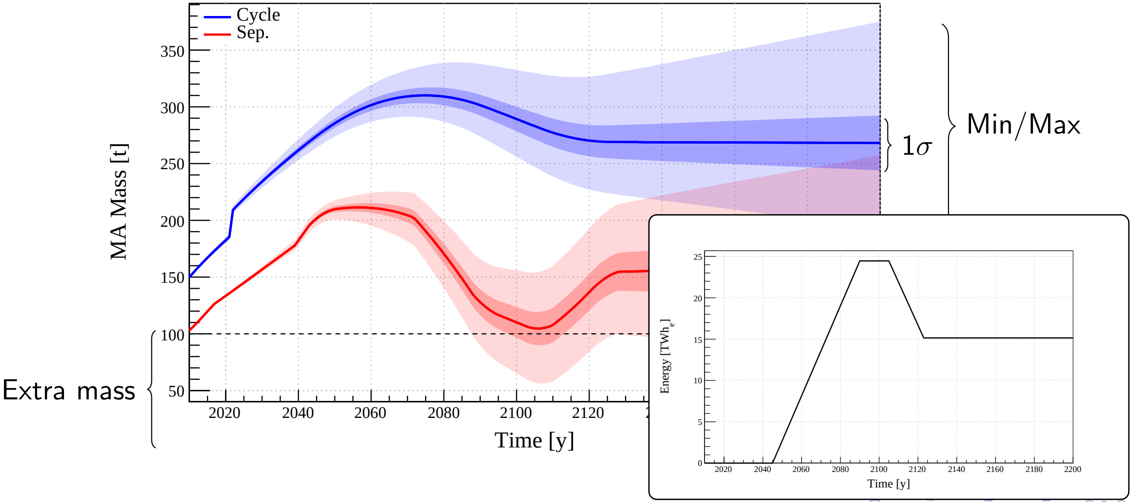
TR_EVOL

- Simulation of all facilities
- Mass and isotopic composition of the selected streams along the cycle
- ORIGEN for decay and irradiations

ROOT framework

- Data processing


Cycle
Sep.
350
300
250
200
150
100
50
MA Mass [t]
2020
2040
2060
2080
2100
2120
2140
2160
2180
2200
Time [y]
1σ
Min/Max
Extra mass


Cycle
Sep.
MA Mass [t]
Time [y]
1σ
Min/Max
Extra mass
Energy [TWh_e]
Time [y]

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	Variables	Sign	η_i	S_i	ST_i	$ST_i - S_i$		Variables	Sign	η_i	S_i	ST_i	$ST_i - S_i$
MA pool	Pu_{ADS}	+	0.33	0.30	0.30	0.00	MA cycle	E_{PWR}	+	0.32	0.33	0.35	0.02
	E_{PWR}	+	0.25	0.27	0.27	0.01		Pu_{ADS}	+	0.27	0.23	0.23	0.00
	ε_{ADS}	+	0.21	0.20	0.20	0.00		ε_{ADS}	+	0.16	0.15	0.15	0.00
	ε_{UOX}	−	0.09	0.08	0.08	0.00		ε_{UOX}	−	0.11	0.10	0.10	0.00
	Q_{UOX}	+	0.06	0.05	0.05	0.00		Q_{UOX}	+	0.07	0.06	0.06	0.00
	ε_{MOX}	−	0.03	0.05	0.06	0.01		ε_{MOX}	−	0.04	0.06	0.08	0.02
	r_{MOX}	+	0.03	0.04	0.05	0.01		r_{MOX}	+	0.03	0.05	0.07	0.02
Pu pool	ε_{UOX}	−	0.44	0.42	0.41	−0.01	Pu cycle	ε_{UOX}	−	0.45	0.45	0.44	−0.01
	r_{MOX}	−	0.19	0.22	0.22	0.00		r_{MOX}	−	0.17	0.19	0.18	0.00
	ε_{MOX}	+	0.13	0.16	0.16	0.00		Q_{UOX}	−	0.13	0.13	0.13	−0.01
	Q_{UOX}	−	0.12	0.12	0.12	−0.01		ε_{MOX}	+	0.12	0.13	0.13	0.00
	E_{PWR}	+	0.09	0.07	0.07	0.00		E_{PWR}	+	0.12	0.11	0.11	−0.01
	Pu_{ADS}	−	0.03	0.03	0.03	−0.01		Pu_{ADS}	−	0.02	0.03	0.02	−0.01
	ε_{ADS}		0.00	0.01	0.00	−0.01		ε_{ADS}		0.00	0.01	0.00	−0.01

Polynomial chaos expansion

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Orthogonal polynomials expansion

$$\left.\begin{array}{c} Y = \sum \alpha_{\boldsymbol{\mu}} \Psi_{\boldsymbol{\mu}}(\boldsymbol{X}) \\ \langle \Psi_{\boldsymbol{\mu}} | \Psi_{\boldsymbol{\nu}} \rangle = \int d\boldsymbol{x}\, \Psi_{\boldsymbol{\mu}}(\boldsymbol{x}) \Psi_{\boldsymbol{\nu}}(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x}) = \left\| \Psi_{\boldsymbol{\mu}} \right\|^2 \delta_{\boldsymbol{\mu}\boldsymbol{\nu}} \end{array}\right\} \quad \alpha_{\boldsymbol{\mu}} = \frac{\langle Y | \Psi_{\boldsymbol{\mu}} \rangle}{\left\| \Psi_{\boldsymbol{\mu}} \right\|^2}$$

Distribution	Polynomials
Uniform	Legendre
Normal	Hermite
Gamma	Laguerre
Beta	Jacobi

$$\Psi_{\boldsymbol{\mu}}(\boldsymbol{X}) = \prod_{i=1}^{d} \psi_i^{(p_i)}(X_i) \qquad \boldsymbol{\mu} = \{p_1, \ldots, p_d\}$$

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^{d} f_{X_i}(x_i)$$

Statistical moments

$$\left(\widehat{\alpha}_{\boldsymbol{\mu}} \equiv \alpha_{\boldsymbol{\mu}} \left\|\Psi_{\boldsymbol{\mu}}\right\|^2\right)$$

$$\mathbb{E}\left[Y\right] = \widehat{\alpha}_{\mathbf{0}} \quad \mathrm{Var}\left[Y\right] = \sum_{\boldsymbol{\mu}\neq\mathbf{0}} \widehat{\alpha}_{\boldsymbol{\mu}}$$

First and total Sobol indices

$$S_i = \sum_{\boldsymbol{\mu}\in\mathcal{I}_i} \widehat{\alpha}^2_{\boldsymbol{\mu}} \Big/ \mathrm{Var}\left[Y\right] \qquad \mathcal{I}_i = \left\{\boldsymbol{\mu} \in \mathbb{N}^d : \mu_i > 0,\ \mu_{i\neq j} = 0\right\}$$

$$ST_i = \sum_{\boldsymbol{\mu}\in\mathcal{I}_i} \widehat{\alpha}^2_{\boldsymbol{\mu}} \Big/ \mathrm{Var}\left[Y\right] \qquad \mathcal{I}_i = \left\{\boldsymbol{\mu} \in \mathbb{N}^d : \mu_i > 0\right\}$$

Other terms for free

$$S_{i_1,\dots,i_s} = \sum_{\boldsymbol{\mu}\in\mathcal{I}_{i_1,\dots,i_s}} \widehat{\alpha}^2_{\boldsymbol{\mu}} \Big/ \mathrm{Var}\left[Y\right] \qquad \mathcal{I}_{i_1,\dots,i_s} = \left\{\boldsymbol{\mu} \in \mathbb{N}^d : k \in \{i_1,\dots,i_s\} \Leftrightarrow \mu_k > 0\right\}$$

The infinite series has to be truncated at certain order $p = \sum \alpha_i \implies \binom{d+p}{p}$ terms

$$Y(\boldsymbol{X}) = \sum_{\boldsymbol{\mu}} \alpha_{\boldsymbol{\mu}} \Psi_{\boldsymbol{\mu}}(\boldsymbol{X}) \approx \sum_{\boldsymbol{\mu}=\boldsymbol{0}}^{p} \alpha_{\boldsymbol{\mu}} \Psi_{\boldsymbol{\mu}}(\boldsymbol{X}) \equiv Y'(\boldsymbol{X})$$

Minimization problem

$$\widehat{\boldsymbol{\alpha}} = \arg \min \mathbb{E}\left[\left(Y - Y'\right)^2\right] = \left(\boldsymbol{\Phi}^\intercal \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^\intercal \mathcal{Y}$$

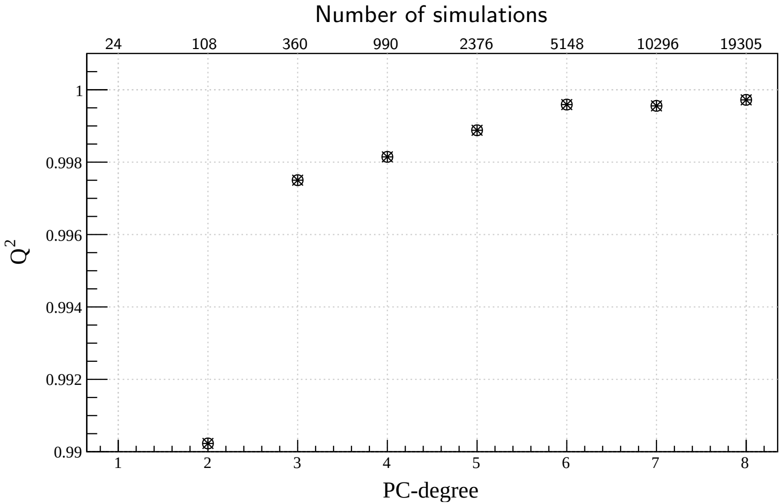
$$\left(\mathcal{Y} = \left\{Y(\boldsymbol{x}^{(1)}), \dots, Y(\boldsymbol{x}^{(N)})\right\}^\intercal \quad \boldsymbol{\Phi}_{ij} = \Psi_j(\boldsymbol{x}^{(i)})\right)$$

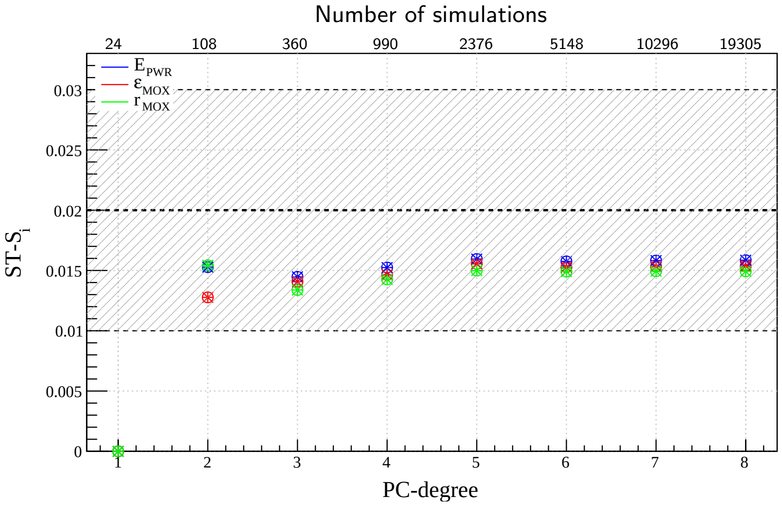
Leave-One-Out Cross-Validation (LOOCV) error estimation

$$\varepsilon_{LOO} = \frac{1}{N}\sum\left(Y(\boldsymbol{X}^{(i)}) - Y'(\boldsymbol{X}^{(\sim i)})\right)^2 = \frac{1}{N}\sum\left(\frac{Y(\boldsymbol{X}^{(i)}) - Y'(\boldsymbol{X}^{(i)})}{1-d_i}\right)^2$$

$$\boldsymbol{d} = \mathrm{diag}(\Phi(\Phi^\intercal\Phi)^{-1}\Phi^\intercal)$$

$$Q^2 = 1 - \frac{\varepsilon_{LOO}}{\mathrm{Var}\left[y\right]}$$


Number of simulations
24
108
360
990
2376
5148
10296
19305
1
0.998
0.996
0.994
0.992
0.99
Q^2
1
2
3
4
5
6
7
8
PC-degree


Number of simulations
24
108
360
990
2376
5148
10296
19305
E_{PWR}
ε_{MOX}
r_{MOX}
ST-S_i
0.03
0.025
0.02
0.015
0.01
0.005
0
1
2
3
4
5
6
7
8
PC-degree

Looking for interactions

- Let $1 \equiv E_{\text{PWR}}, \quad 2 \equiv \varepsilon_{\text{MOX}}, \quad 3 \equiv r_{\text{MOX}}$

$$\underbrace{\begin{aligned} S_1 &= 0.33 \\ S_2 &= 0.06 \\ S_3 &= 0.05 \end{aligned} \qquad \begin{aligned} ST_1 &= 0.35 \\ ST_2 &= 0.08 \\ ST_3 &= 0.07 \end{aligned}}_{\substack{\text{Direct integration} \\ \text{112500 simulations}}} \qquad \underbrace{\begin{aligned} S_{12} &= 0.006 \\ S_{13} &= 0.006 \\ S_{23} &= 0.006 \end{aligned} \qquad S_{123} = 0.003}_{\substack{\text{Chaos expansion 4th degree} \\ \text{990 simulations}}}$$

Conclusions

- Sobol indices provide a lot of information but very expensive
- Dimension reduction with cheaper methodology (*e.g.* sensitivity analysis)
- Quasirandom sequences provide better convergence than pseudorandom numbers
- Surrogate models may reduce the number of simulations

But...

- How can the error in the Sobol indices be estimated?