Nuclear data and fuel cycles

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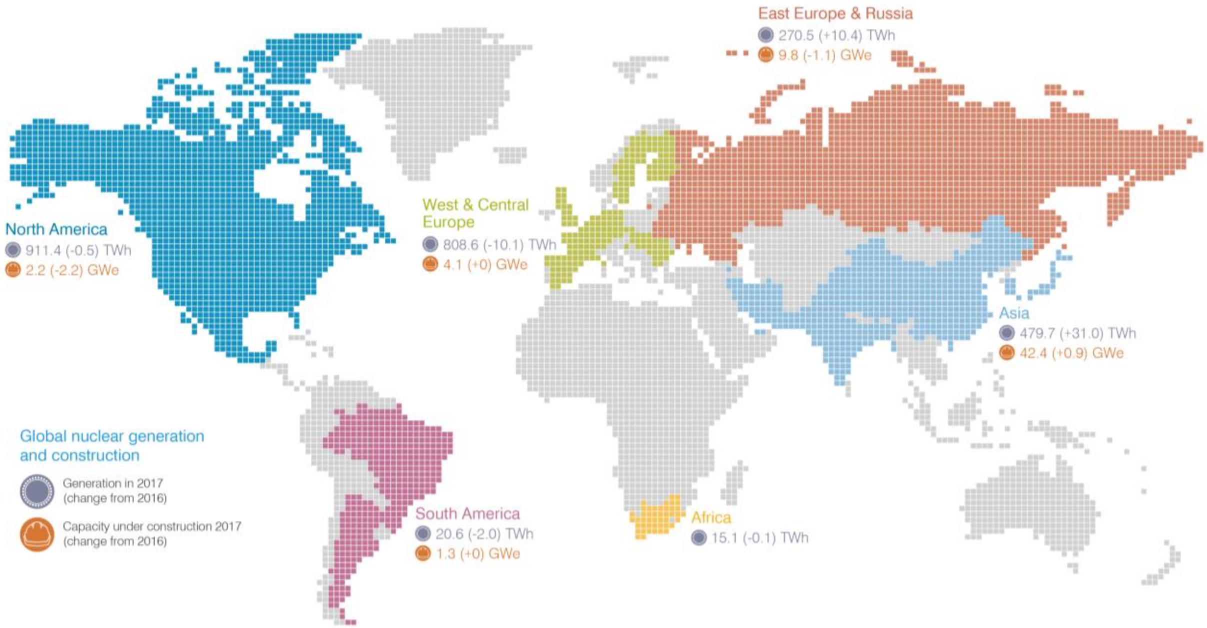
- Generation of electricity is one of the main applications of the technology of nuclear fission.
- Currently, there are ~440 reactors in operation in the world, with 52 more in construction (Asia ↑↑), representing ~11.5% of the global energy consumption.
- In Spain, there are 7 reactors in operation (Almaraz I & II, Ascó I & II, Trillo, Cofrentes, Vandellós II).



Source: World Nuclear Association 2017

What is a nuclear fuel cycle?

Nuclear fuel cycle studies cover all the processes involved in the production of energy from nuclear materials: from mining to final disposal

The activities are usually classified in two stages:

- **Front-end**, activities for the preparation of the fuel for its irradiation (mining, conversion, enrichment, fabrication)
- **Back-end**, activities for the safe management of spent nuclear fuel (reprocessing, disposal)

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- Introduction. What is a nuclear fuel cycle?
- **Types of fuel cycles**
- Nuclear fuel cycle calculations
- Propagation of uncertainties along the fuel cycle
- Impact of nuclear data and uncertainties in the fuel cycle assessment
- Nuclear fuel cycle optimization

Types of fuel cycles

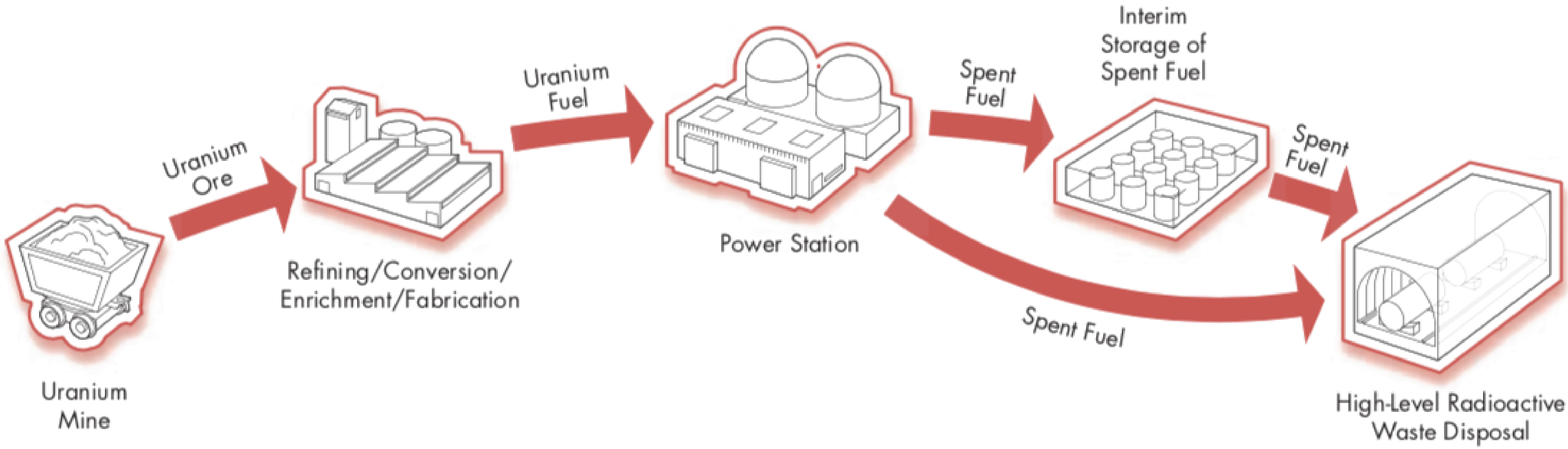
Based on the flows of materials

- ***Open fuel cycles***
- ***Closed fuel cycles***

Based on the flows of materials

- ***Open fuel cycles***
- ***Closed fuel cycles***

No recycling of the materials

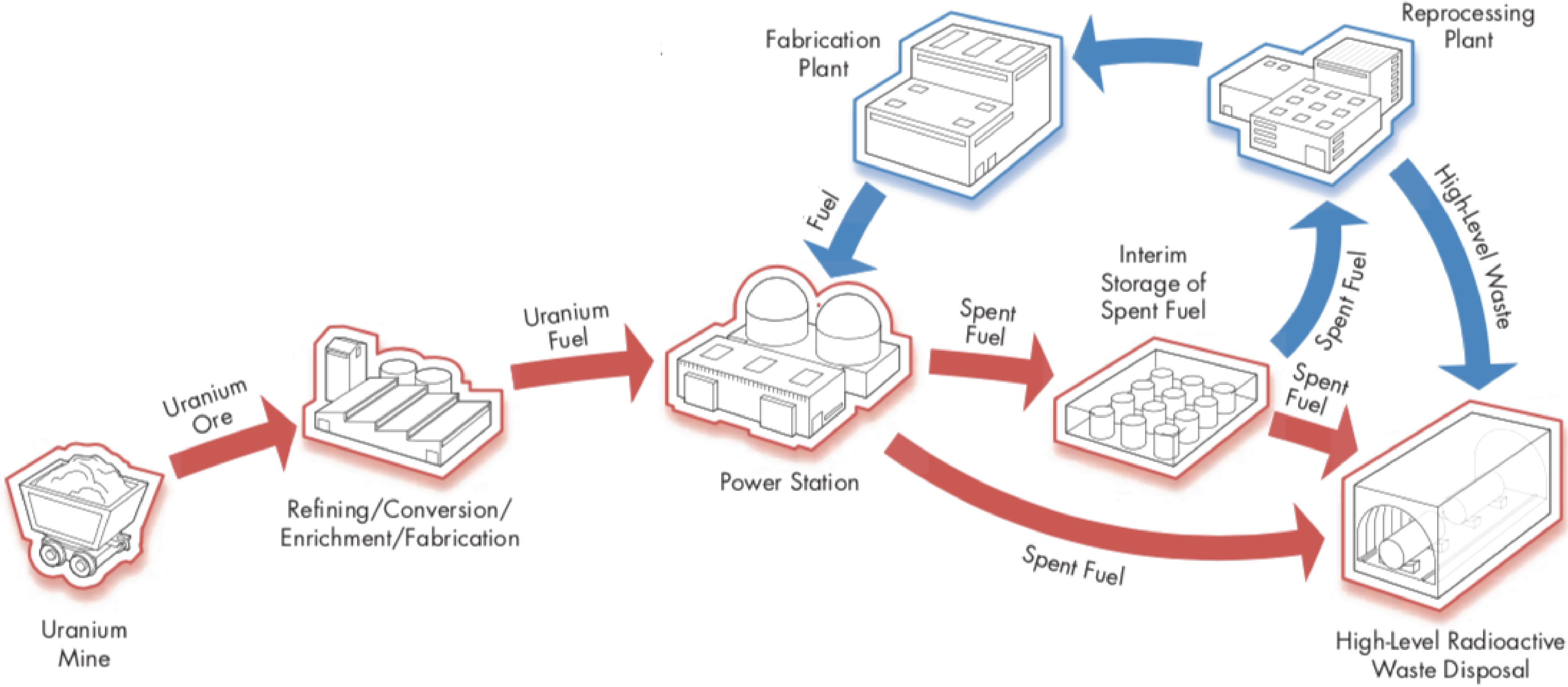


A. Clamp, Towards and Integrated Fuel Cycle, 2008

Based on the flows of materials

- *Open fuel cycles*
- ***Closed fuel cycles***

Materials are recycled/multi-recycled in the reactors before their final disposal



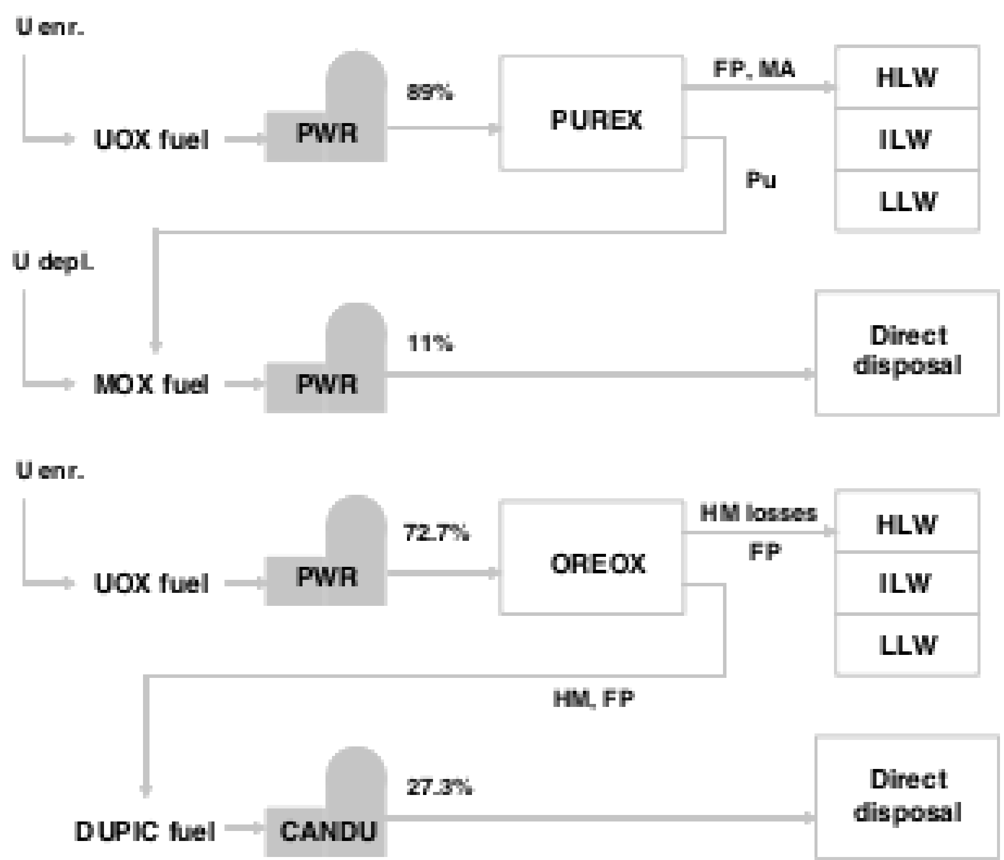
A. Clamp, Towards and Integrated Fuel Cycle, 2008

More detailed classification: Single recycling

Pu recycled once in LWR with MOX.

Np can also be included to avoid the separation of pure Pu.

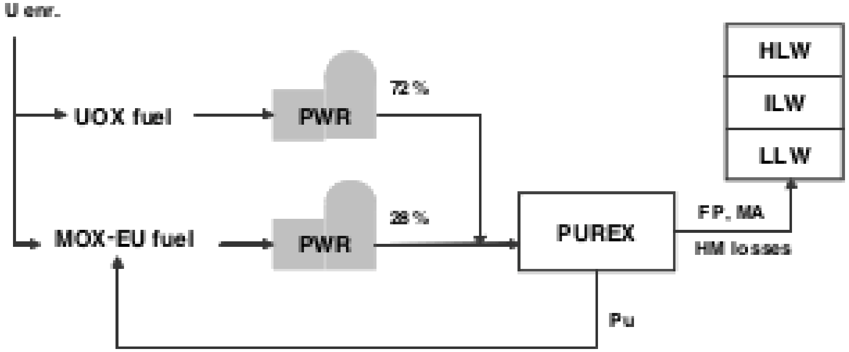
Recycle of U.

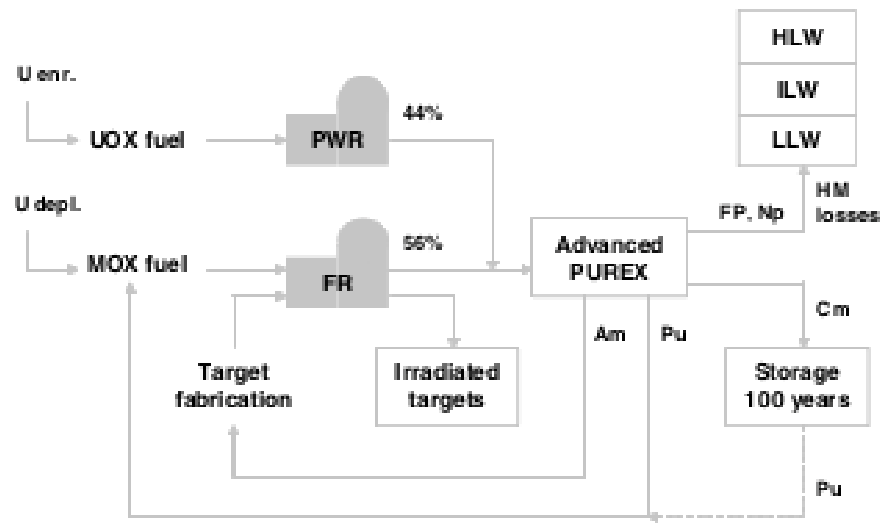


OECD/NEA. *Advanced Nuclear Fuel Cycles and Radioactive Waste Management*. 2006, 10.1787/9789264024861-en

More detailed classification: Partially closed

Pu (an eventually Am and Cm) is continuously recycled, either in PWR or FR

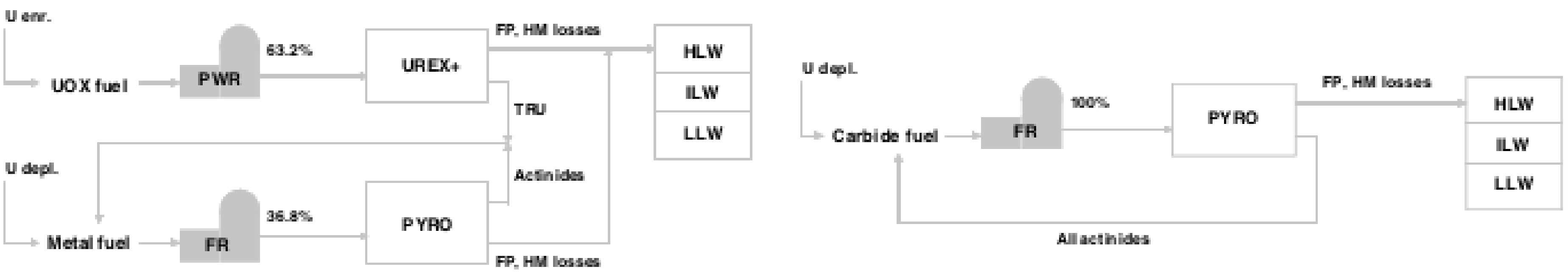




OECD/NEA. *Advanced Nuclear Fuel Cycles and Radioactive Waste Management*. 2006, 10.1787/9789264024861-en

More detailed classification: Fully closed

All actinides are continuously recycled in advanced reactors until their fission



OECD/NEA. *Advanced Nuclear Fuel Cycles and Radioactive Waste Management*. 2006, 10.1787/9789264024861-en

Even more detailed classification!

Note that the previous classification only focuses on waste management.

Based on how they are implemented, a fully closed can be:

- Double strata, two well differentiated fleets, one dedicated to energy production while the other focuses on TRU burning
- Mixture of Fast Reactors and LWR
- Only Fast Reactors

Benefits of advanced fuel cycles:

- Radiotoxicity reduction
- Optimization of natural resources
- Better energy recovery
- Waste minimization & management
- Proliferation resistance
- Economic competitiveness

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The need of simulators

These studies require following materials flows between different facilities.

- A large number of isotopes has to be tracked
- And as more installations are considered, the complexity of the cycle grows
- In 2014, U.S. DOE conducted an screening study covering 4398 different configurations! (https://fuelcycleevaluation.inl.gov/SitePages/Home.aspx)

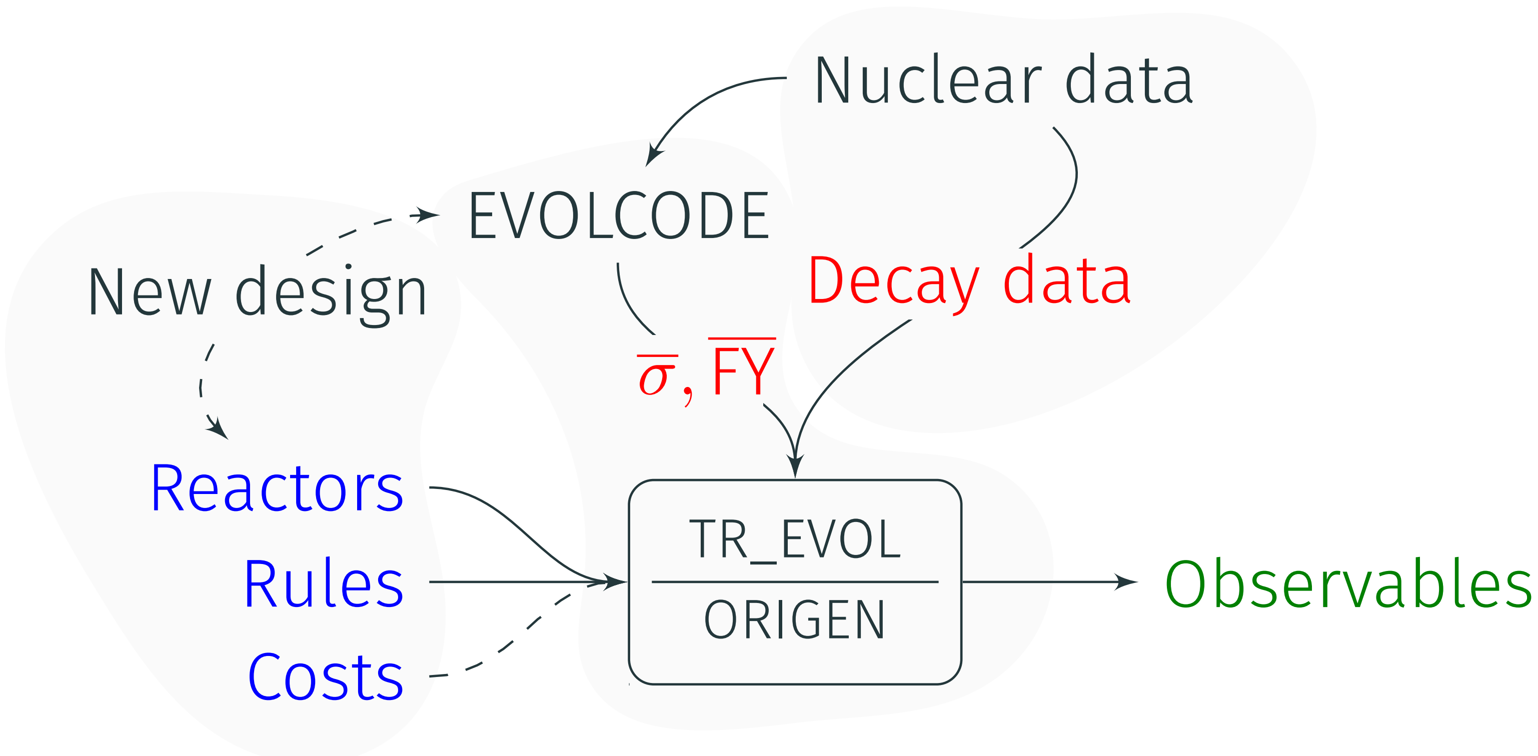
Computer codes!

Fuel cycle simulators

Code	Institution	Country	Code	Institution	Country
ANICCA	SCK·CEN	Belgium	FUTURE	KAERI	South Korea
CAFCA	MIT	US	GENIUS	UW	US
CEPMNFC	Cornell Univ.	US	JOSETTE	BME	Hungary
CLASS	CNRS/IRSN	France	MARKAL	BNL	US
COSAC	AREVA	France	NFCSim	LANL	US
COSI6	CEA	France	NFCSS	IAEA	---
CYCLE	IPPE	Russia	NUWASTE	NWTRB	US
CYCLUS	US	US	NMB	JAEA	Japan
DANESS	ANL	US	ORION	NNL	UK
DESAE 2.2	Kurchatov Inst.	Russia	SITON	BME	Hungary
DYMOND	ANL	US	TIRELIRE-ST.	EDF	France
FANCSEE	KTH	Sweden	TR_EVOL	CIEMAT	Spain
FAMILY 21	JAEA	Japan	VISION	INL	US

Anatomy of a simulator

In general, all of them work in a similar way



OECD/NEA benchmark on TRU management

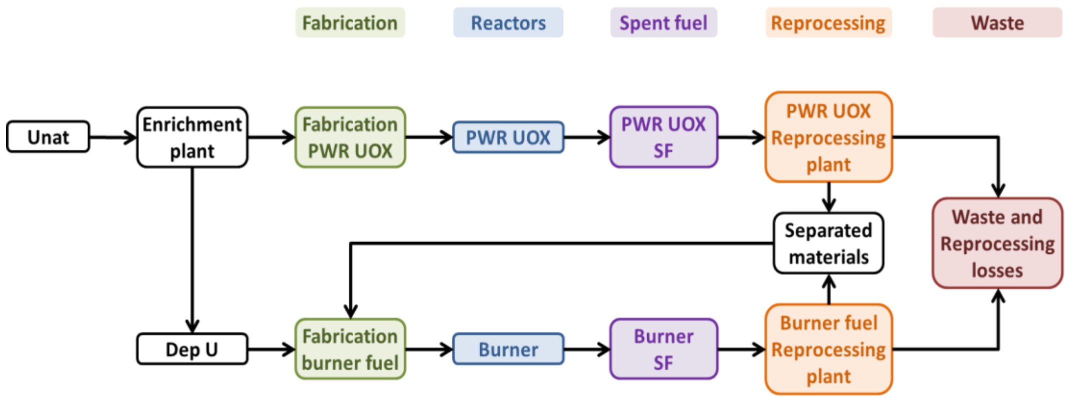
Compare codes and models;

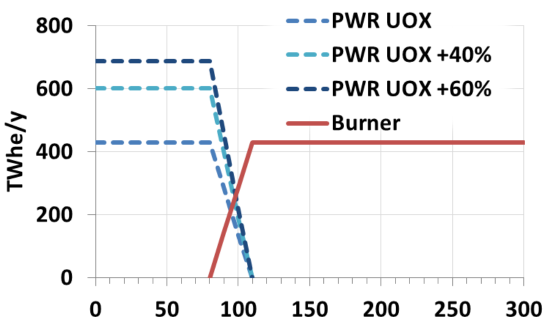
Evaluate how much of the materials in spent fuel can be burnt with different “burner fleets”;

Assess the possibility of going back to an equilibrium state after the reduction of the TRU stocks.

Three steps scenarios:

- Step 1: equilibrium PWR UOX fleet
- Step 2: reduction of the TRU inventories with a burner fleet
- Step 3: evolution toward a sustainable state (e.g. stabilization of the Pu inventory).





OECD/NEA benchmark: Expected results

Reactors:
- Pu, Am, Np, Cm and MA contents (wt%)
- Pu, Am, Np, Cm and MA balances (kg/TWhe)

Enrichment plant:
- Natural uranium consumption (t and t/y)
- Enriched uranium need (SWU and t/y)

Fabrication and reprocessing plants:
- Annual flow (t/y)
- Pu, Am, Np, Cm annual flows (t/y)
- Activities (Bq and Bq/t)
- Radiotoxicity (Sv and Sv/t)
- Decay heat (W and W/t)

Separated materials storage:
- Stored mass for each separated material (t)

Material transportation:
- Annual flow (t/y)
- Neutron emissions (n/s and n/s/t)
- Decay heat (W and W/t)

Disposals:
- Mass of waste (t)
- Long term radiotoxicity of waste accumulated at the end of the scenario (Sv, over 1.10^6 years)

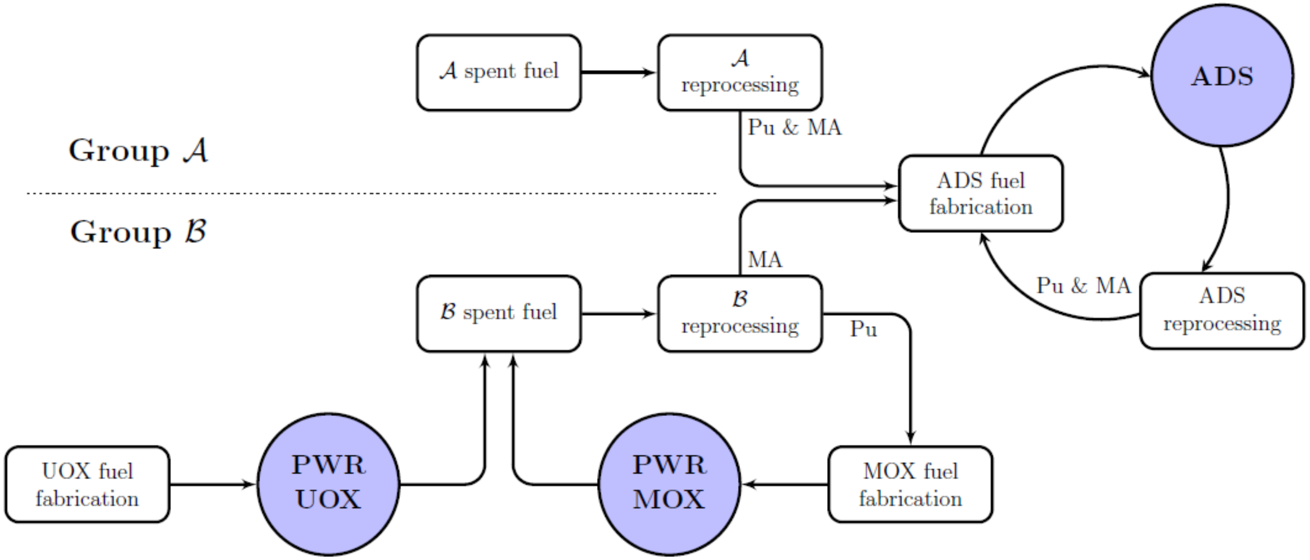
Inventories:
- Pu, Am, Np, Cm and MA inventories in cycle (t)
- Pu, Am, Np, Cm and MA inventories in waste (t)
- Pu, Am, Np, Cm and MA total inventories (t)

Contents

UQ: Fuel cycle parameters

Studied for an advanced fuel cycle scenario devoted to the reduction of TRUs.

Two countries collaborate to achieve the objectives.



UQ: Fuel cycle parameters

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	—			

UQ propagation methodologies

Sensitivity coefficients (local)

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

- X First order perturbation
- X Linear and separable variables
- ✓ Fast to compute

Sobol indices (global)

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

- ✓ The whole input parameter space
- ✓ Any kind of dependence
- X High computational demand

Hybrid methodology

UQ results

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

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

Expansion of the response function (the desired observable) into polynomials that are orthogonal within the probability density function of the input variable (the uncertainties) makes the Sobol indices to take an easy form:

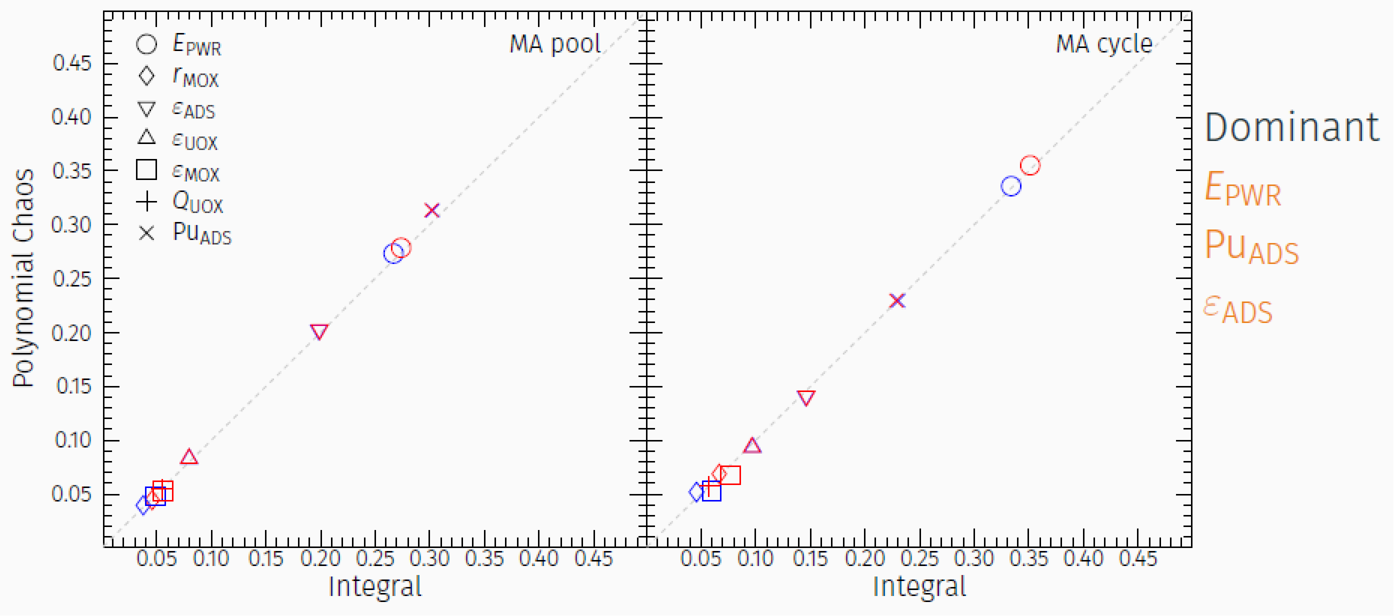
$$\mathcal{F}(X) \approx \sum \alpha_\mu \Psi_\mu(X) \quad \text{for which} \quad \langle \Psi_\mu | \Psi_\nu \rangle := \int dx\, \Psi_\mu(x) \Psi_\nu(x) f_X(x) = \delta_{\mu\nu}$$

The expansion coefficients α_μ can be estimated through regression methods, neglecting non-relevant terms.

Taking advantage of the orthogonal properties, Sobol indices can be calculated only summing over certain elements of the expansion coefficients, and any order coefficient for free!

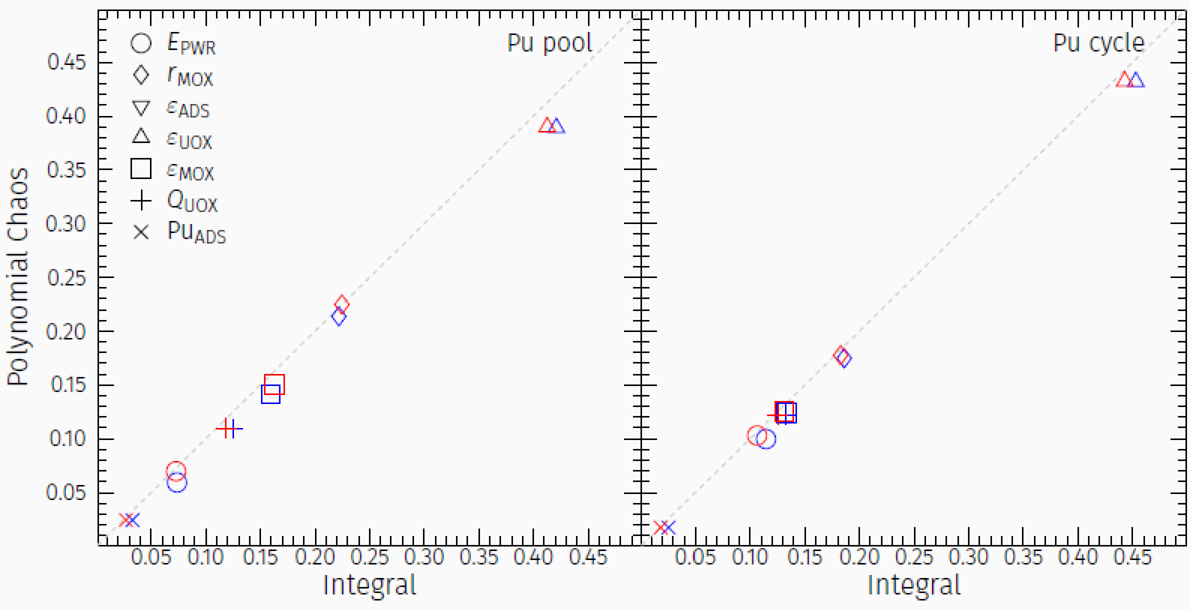
Polynomial chaos expansion

Comparison between direct integration and Polynomial Chaos expansion for first and total order indices for MA streams



Polynomial chaos expansion

Comparison between direct integration and Polynomial Chaos expansion for first and total order indices for Pu streams



Dominant

ε_{UOX}

r_{MOX}

Fuel cycle simulations rely on a large number of parameters that have associated uncertainties.

Cheap sensitivity coefficient methodologies can be coupled with expensive Sobol global methods.

Polynomial Chaos expansion reduce crucially the computational cost:

100 simulations vs 112500

Minutes vs days, at CIEMAT cluster

while obtaining the same results.

Universalization of fuel cycle uncertainties propagation!!!

Any institution with any code in any environment will be able to apply these techniques.

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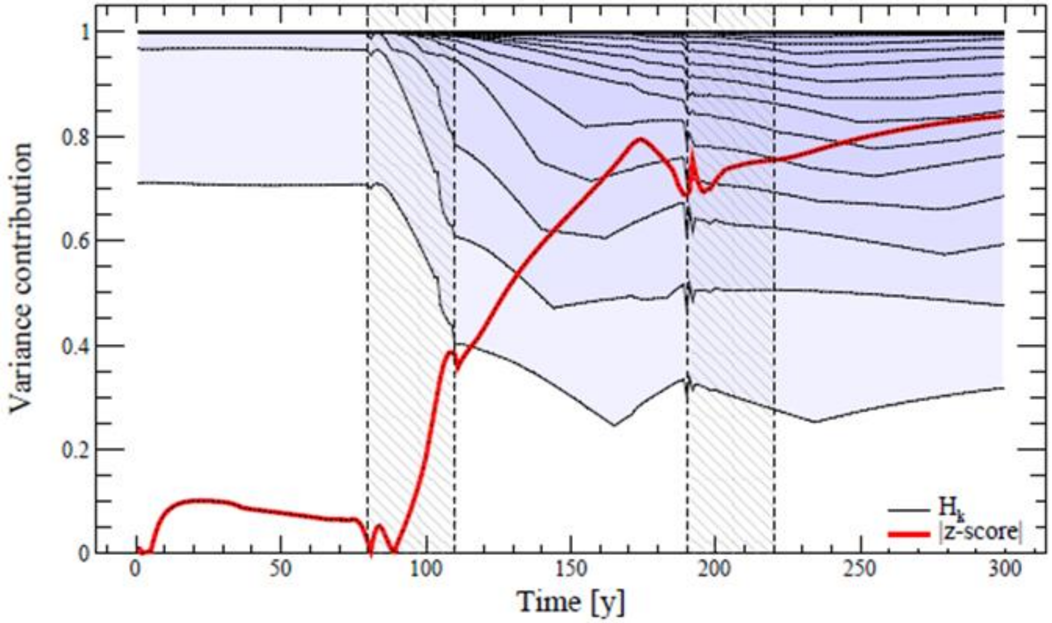
Fuel cycle simulations rely on a large number of parameters that have associated uncertainties.

Other sources of uncertainties exist in fuel cycle calculations:

- Simulator
- Nuclear data

The different uncertainty sources can be compared in separated estimations.

Uncertainties due to the simulator are unavoidable and have to be considered.



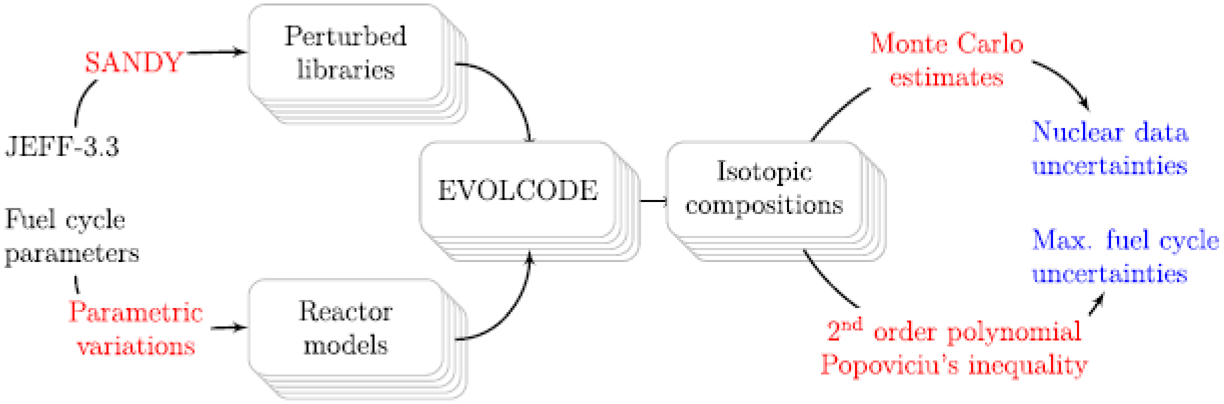
Methodology

The stochastic nuclear data sampling code SANDY has been used to create 1000 perturbed libraries (convergence checked).

In this work, the cross-sections of ^{235,238}U, ^{238,239,240,241}Pu, and ^{241}Am from the JEFF-3.3 nuclear data library have been sampled.

Perturbed files has been verified with the SUMMON code.

A complete Monte Carlo simulation of the burn-up evolution has been performed with EVOLCODE burn-up system for each different perturbed nuclear data library to simulate the irradiation of the PWR pin.



Scenario definition

The Popoviciu's inequality on variances has been used in order to provide an upper limit to the variance produced by fuel cycle parameters:

$$\sigma_i^2 \leq \frac{1}{4}\left(y_i^{max} - y_i^{min}\right)^2$$

Predicting the future

Large deviations in the fuel cycle parameters have been considered.

±5% uncertainty in the fuel cycle parameters.

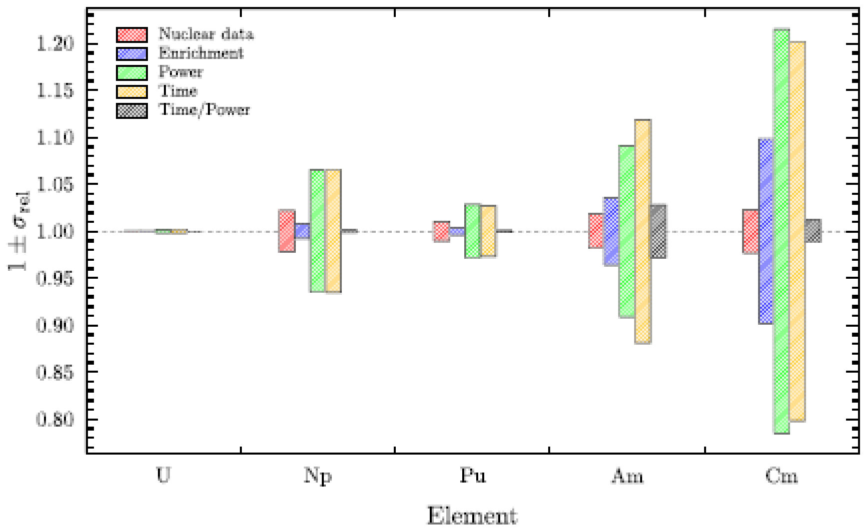
Analyzing the past

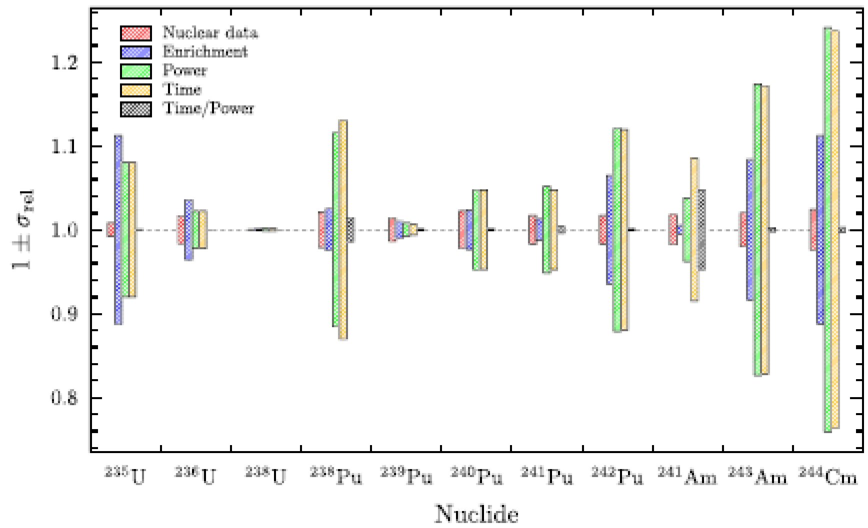
Small deviations in the fuel cycle parameters have been considered.

±0.5% uncertainty in the fuel cycle parameters.

Predicting the future: results

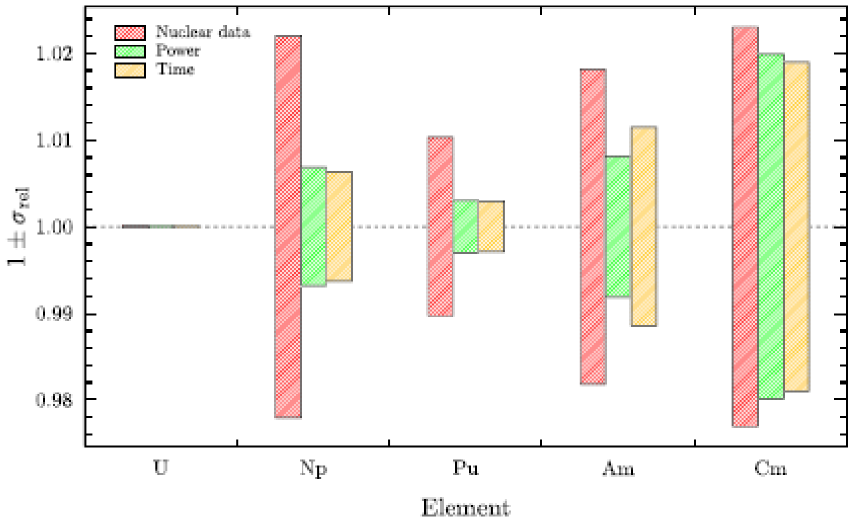
Considered parameters with uncertainty include fuel enrichment, thermal power, irradiation time and a special variation of parameters with unchanged burn-up.

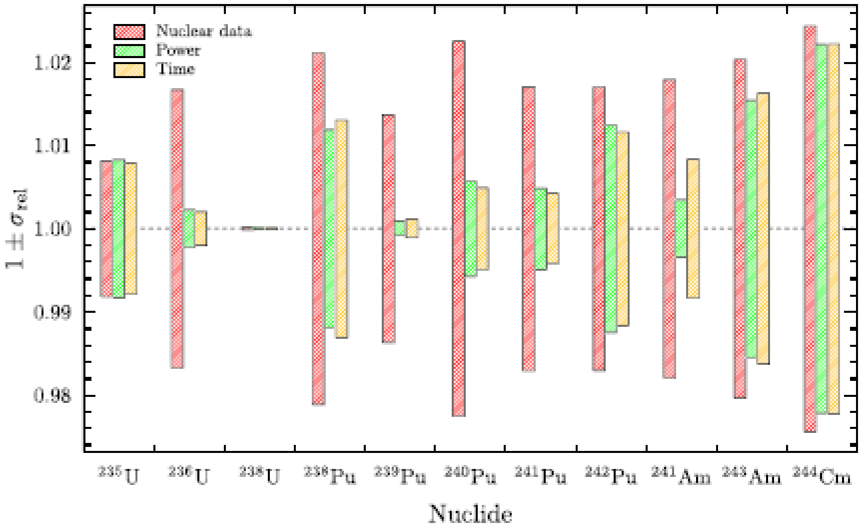




Analyzing the past: results

Considered parameters with uncertainty include fuel enrichment, thermal power and irradiation time.





ND uncertainties

Nuclear data uncertainties have an impact in fuel cycle calculations and cannot be disregarded.

Nowadays, mathematical methodologies exist to assess this impact. Computer power is also available in many institutions.

For future cycles (large uncertainty in fuel cycle parameters), certain isotopes show an uncertainty due to ND similar to that from parameters.

For past cycles (small uncertainty in fuel cycle parameters), ND uncertainty provides the largest contribution.

All these results have been obtained for an open fuel cycle scenario.

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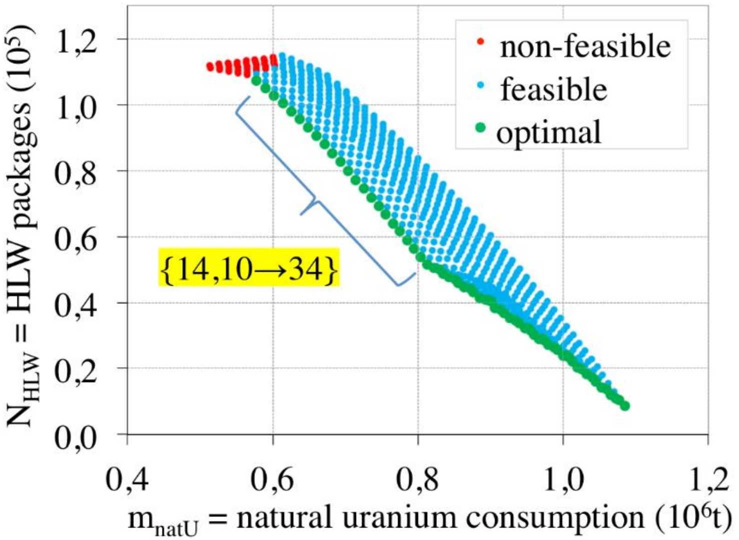
Nuclear fuel cycle optimization is a multiobjective problem

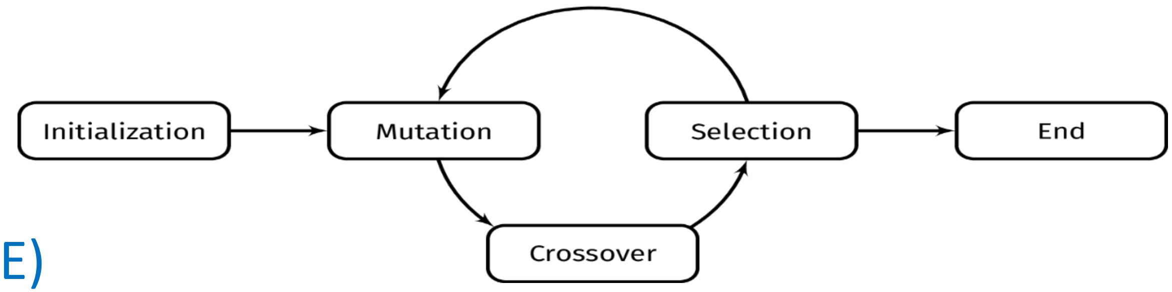
- There are unlimited criteria for the optimization
  - Volume of TRU inventories
  - U_{nat} requirements
  - Fuel cycle costs
  - …
- And in general, no scenario will optimize all of them simultaneously
  - Trade-off between improving one objective and degrading the others: Pareto Front



Freynet, D. et al. "Multiobjective optimization for nuclear fleet evolution scenarios using COSI". In: EPJ Nuclear Sciences & Technologies 2 (2016), p. 9. doi:10.1051/epjn/e2015-50066-7

It also usually contains constrains or restrictions (e.g., the demanded fabrication mass cannot exceed the stocks)

These families of algorithms are based on generating a set of candidate solutions which are iteratively updated until convergence criterion is met.



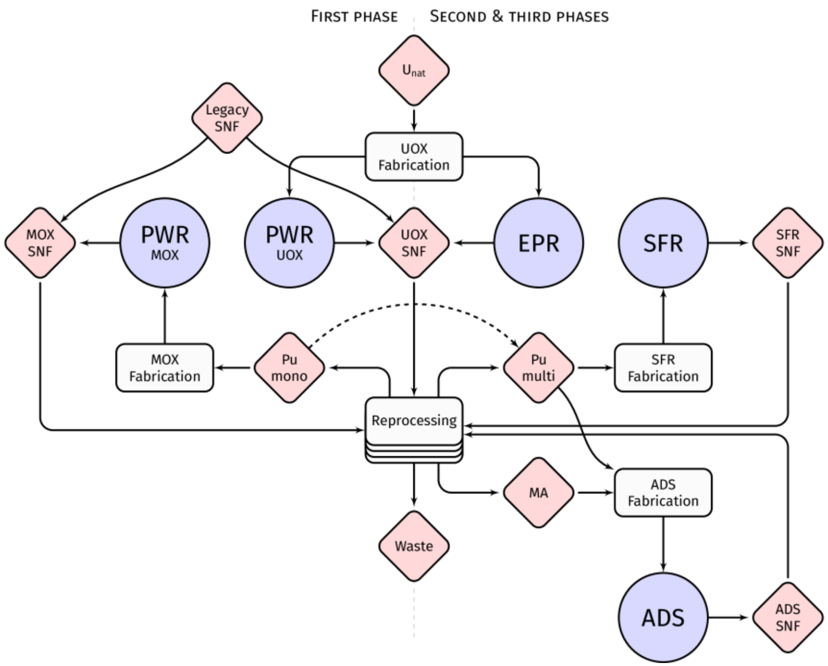
Differential Evolution (DE)

- Extremely simple algorithm
- Three key operations: Mutation, Crossover/Recombination and Selection
    - For every generation, the Mutation and Crossover operators produce a new set of candidate solutions (agents) applying linear combination and permutations to the best ones
    - These candidate solutions are only accepted if they improve the existing ones

Storn, R. and Price, K. Differential Evolution - A simple and efficient adaptive scheme for global optimization over continuous spaces. Tech. rep. TR-95-012. Berlekey: International Computer Science Institute, 1995

Storn, R. and Price, K. "Differential Evolution – A Simple and Efficient Heuristic for global Optimization over Continuous Spaces". In: Journal of Global Optimization 11.4 (1997), pp. 341–359. doi: 10.1023/a:1008202821328

Optimization: Scenario description



Energy fixed at 800 TWhe/year
Reprocessing capacity 2000+800 t_{HM}/year (UOX + MOX)
Uncertainties ±10%

Transition scenario based on CP-ESFR project

- PWR(UOX+MOX) -> EPR + SFR + ADS
  1. Initial phase (2010 – 2040 years)
  2. Burning phase (2040 – 2100)
  3. Stabilization phase (2100 – 2300)
- SFR and ADS energies?
  - Minimize & Stabilize TRU
  - Minimize Cost (capital and O&M~80%)

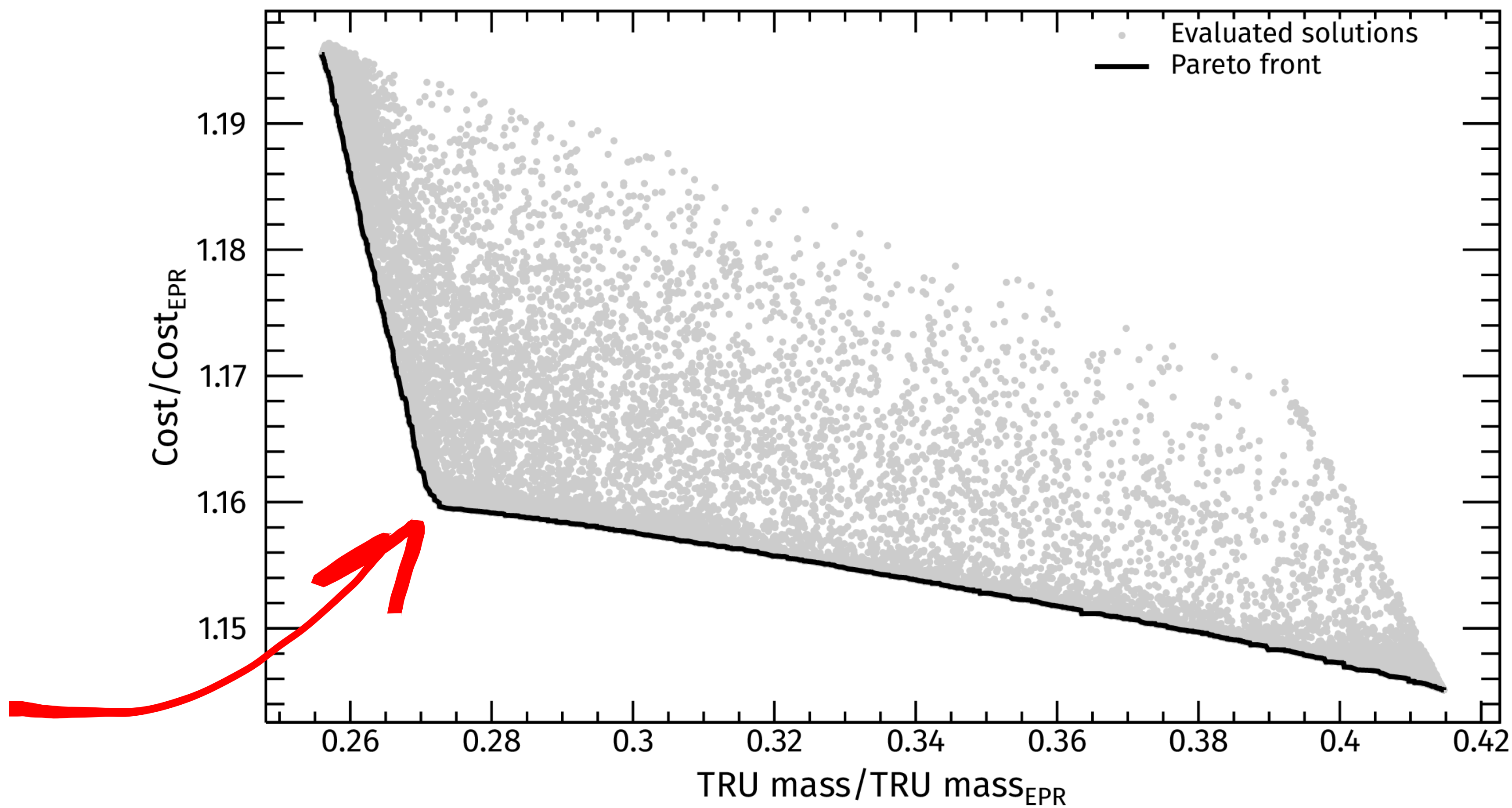
Rodríguez, I. M., et al. "Analysis of advanced European nuclear fuel cycle scenarios including transmutation and economic estimates". In: *Annals of Nuclear Energy* 70 (Aug. 2014), pp. 240–247. 10.1016/j.anucene.2014.03.015.

$$\min_{x \in R^d} (m_{TRU}(\boldsymbol{x}), \mathrm{Cost}(\boldsymbol{x})) \text{ subject to } \begin{cases} \Delta m_{TRU}(\boldsymbol{x}) < 1t \\ m_{External}(\boldsymbol{x}) = 0 \end{cases}$$

(no additional mass)

Optimization: Results

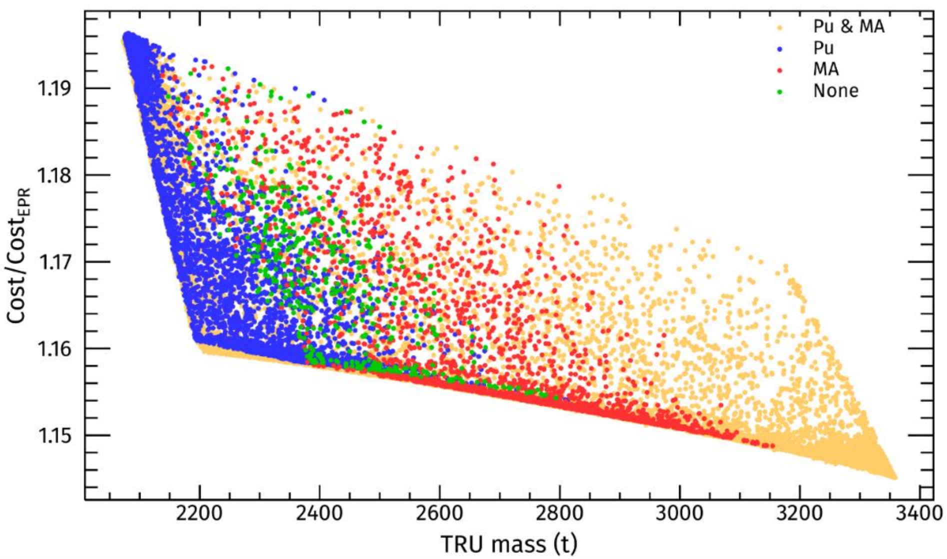
Solutions space: TRU reduction of 60-75% with an extra cost of 15-20%

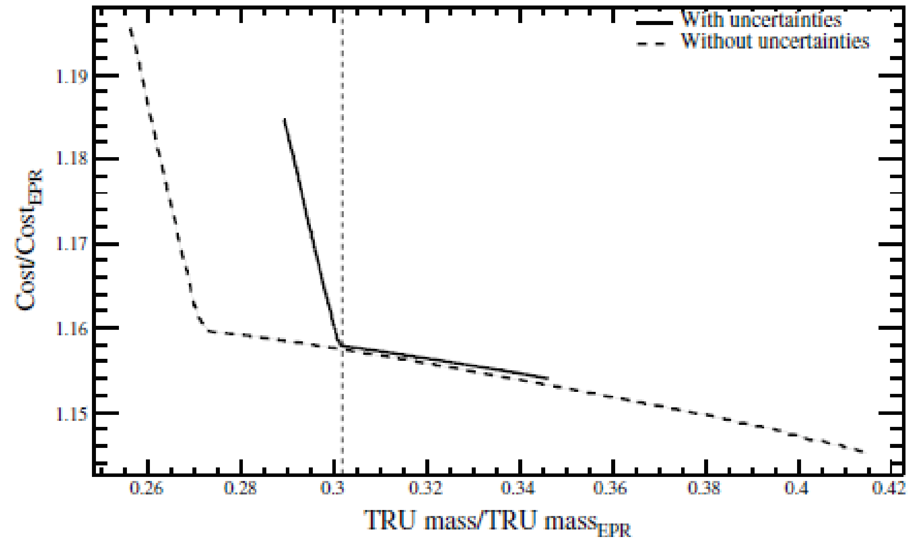


The introduction of the uncertainties (parametric variations) in the Pareto's front scenarios, shows that none of the solutions was robust

- All violates the stabilization constraint
- And a small subset requires an external mass

(those achieving the lower TRU)





Uncertainties should be taken into account during the optimization process!

Final remarks

- Nuclear fuel cycle analyses provide crucial information to decision makers for them to choose the specific fuel cycle of the region/country.
- Nuclear fuel cycle calculations are usually performed with computer codes.
- Uncertainties come from different sources (parameters, simulator, nuclear data) and none can be disregarded.
- Nuclear fuel cycle multiobjective optimization is possible without and with uncertainties but they should be considered from the beginning of the analysis.

Enjoy the school!