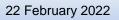
Nuclear data for reactor physics

F. Álvarez-Velarde CIEMAT – Nuclear Innovation Unit





ARIEL-H2020 NuDataPath

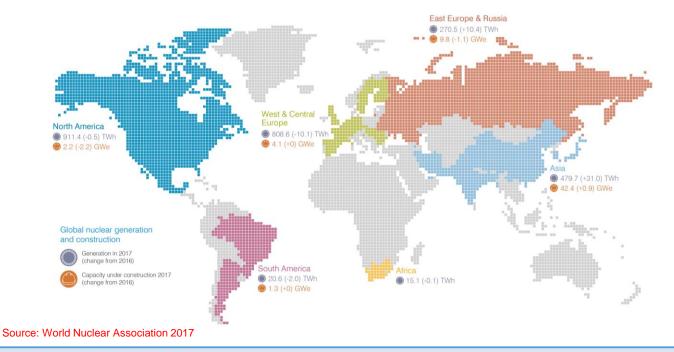
- Introduction
- Role of nuclear data in reactor physics calculations
- Impact of nuclear data and uncertainties in reactor safety parameters and inventory calculations
- Status of actual nuclear data libraries for nuclear reactor applications: strengths and weaknesses

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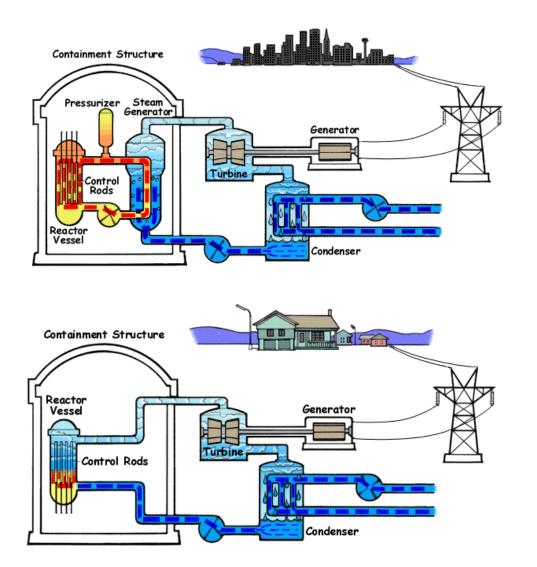
• Introduction

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- Status of actual nuclear data libraries for nuclear reactor applications: strengths and weaknesses

- 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 $\uparrow \uparrow$), 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).



Nuclear reactor



Pressurized water reactor

Boiling water reactor

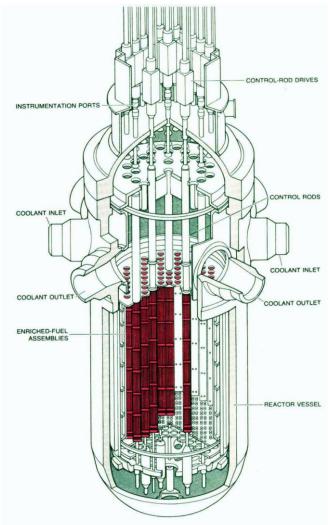
Nuclear reactor

• The nuclear power plant generates energy in the same way as other power plants.

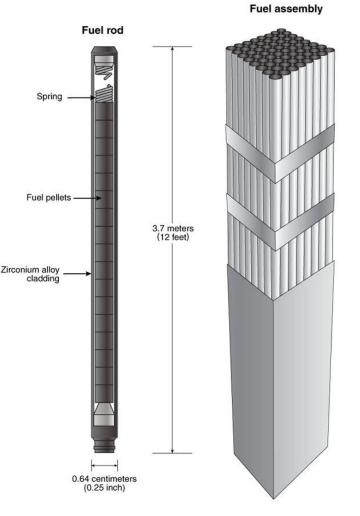
- The idea is to heat water to create steam.
- The steam moves a turbine and electricity is then generated.
- The nuclear power plant heats water by means of nuclear fission reactions.
- A chain reaction is maintained in a controlled manner.
- The reactor core is formed by fuel elements assembled in fuel assemblies containing a number of fuel rods.

$$Q_f = \overline{E_K} + \overline{E_{np}} + \overline{E_{\gamma p}} + \overline{E_\beta} + \overline{E_{nd}} + \overline{E_{\gamma d}} + \overline{E_{\overline{\gamma}}}$$

Nuclear reactor



Nuclear reactor



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- Impact of nuclear data and uncertainties in reactor safety parameters and inventory calculations
- Status of actual nuclear data libraries for nuclear reactor applications: strengths and weaknesses

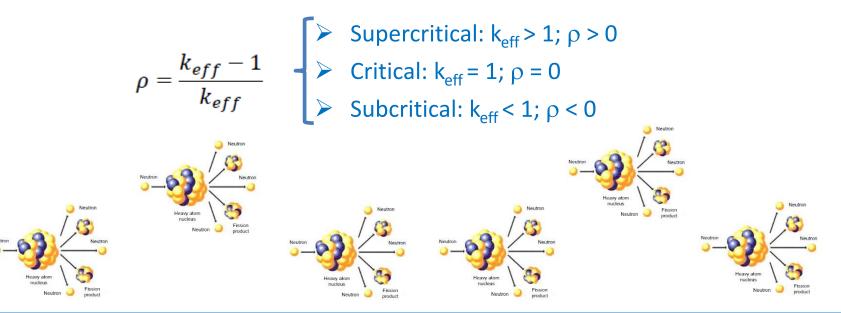
- The goal is the characterization of the reactor core.
- Neutron transport -> Boltzmann equation.
- Neutron flux: defined as the total length travelled by all free neutrons per unit time and volume.

$$\frac{1}{v} \frac{\partial \Phi(\vec{r}, E, t)}{\partial t} + \vec{\Omega} \cdot \vec{\nabla} \Phi(\vec{r}, E, t) = S(\vec{r}, E, t) - \Sigma_T(\vec{r}, E, t) \Phi(\vec{r}, E, t) + \int_0^\infty \Sigma_s(\vec{r}, E', t') f(\vec{r}, E' \to E, t) \Phi(\vec{r}, E', t) dE' + \int_0^\infty s(E') \Sigma_f(\vec{r}, E', t') v(E', t) \Phi(\vec{r}, E', t) dE'$$

• The equation is a balance between neutron production and neutron losses.

$$\stackrel{\text{Simplifying}}{\longrightarrow} \frac{1}{v} \frac{\partial \phi}{\partial t} = D \nabla^2 \phi(\vec{r}, t) - \Sigma_a \phi(\vec{r}, t) + \frac{v \Sigma_f}{k_{eff}} \phi(\vec{r}, t)$$

- *k_{eff}* is introduced in the equations to study how far the reactor is from critical. It
 is defined as the amount of neutrons in one generation over the amount of
 neutrons in the previous generation.
- Concept of reactivity:



Delayed neutrons and delayed neutron fraction β_{eff}

- Most (>99%) of the neutrons emitted in the fission process are emitted at virtually the same time of the fission themselves → *prompt neutrons*.
- The balance is emitted at later times as the result of the decay of short-lived fission products → *delayed neutrons*.
- Delayed neutron information is usually provided in a number of delayed neutron groups (6-8).
- The total number of delayed neutrons emitted is known as the *delayed neutron fraction* (β). Usually the concept used is the *effective delayed neutron fraction* (β_{eff})
- Information about the number prompt and delayed neutrons is included in the ENDF format (MF=5):
 - MT=455: Nubar delayed ($\bar{\nu}_d$).
 - MT=456: Nubar prompt ($\bar{\nu}_p$).
 - MT=452: Nubar total (\bar{v}_t).

Delayed neutrons and delayed neutron fraction β_{eff}

- Delayed neutrons play a prominent role in reactor dynamics to make a reactor controllable.
- Point kinetics equations:

$$\frac{\partial n(t)}{\partial t} = \frac{\rho - \beta_{eff}}{\Lambda_{eff}} n(t) + \sum_{j} \lambda_{j} c_{j}(t) + S_{ext}(t)$$
$$\frac{\partial c_{j}(t)}{\partial t} = -\lambda_{j} c_{j}(t) + \frac{1}{\Lambda_{eff}} \beta_{eff,j} n(t)$$

• The solution of these equations usually takes the shape:

$$n(t) = C_0 \cdot exp\left(\frac{\rho - \beta_{eff}}{\Lambda_{eff}}\right) + \sum_j C_j \cdot exp\left(-\frac{\lambda_j \rho}{\rho - \beta_{eff}}\right)$$

- If $\rho > \beta_{eff}$ (prompt supercritical) reactor dynamics is dominated by prompt neutrons.
- If $0 < \rho < \beta_{eff}$ (supercritical but delayed subcritical) reactor dynamics is dominated by delayed neutrons.

- The safety of the nuclear reactor is also measured with reactivity safety coefficients:
 - Doppler coefficient: defined as a relation between fuel temperature changes and reactivity changes in the nuclear reactor core.

$$K_D = \frac{\rho_{nom} - \rho_{pert}}{\ln(\frac{T_{nom}}{T_{pert}})}$$

- Void coefficient: defined as a relation between the creation of voids (typically bubbles in the coolant leading to density changes) and reactivity changes in the nuclear reactor core.
- The effective neutron generation time, $\Lambda_{\rm eff}$: average time spent by one neutron until producing another. Needed in the PK equations.

- Other reactivity safety coefficients:
 - Control rod worth: change in reactivity produced by the motion of the control rods.
 - Shutdown margin: instantaneous amount of reactivity by which the reactor would be subcritical from its present condition assuming all full-length rod cluster assemblies (shutdown and control) are fully inserted (excepting one).
 - Power coefficient: defined as a relation between the difference in temperature between fuel and moderator (caused by power), and reactivity changes in the nuclear reactor core. Also the fission product poisoning has an effect in this coefficient.

- Long-term change of the material due to exposure to radiation.
 - Described by the Bateman equations.

$$\frac{dn_i(\vec{r},t)}{dt} = \left[\sum_{j\neq i} n_j(\vec{r},t) \left(\lambda_{ji} + \int \sigma_{ji}(\vec{r},E) \Phi(\vec{r},E,t) dE\right)\right] - \left[n_i(\vec{r},t) \left(\lambda_i + \int \sigma_{abs}(\vec{r},E) \Phi(\vec{r},E,t) dE\right)\right]$$

• It includes the consumption of the nuclear fuel and the creation of new actinides and poisoning fission products affecting the reactivity of the system.

Introduction

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Types of problems to solve:

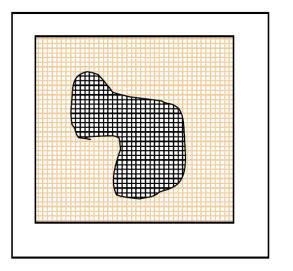
- Transport of neutrons, photons and other particles through the reactor
 - Map of the neutron flux
 - Radiation crossing a shielding element (dose, probability, damage,...)
 - Neutron energy spectra, dependence vs. time of the neutron flux at a point,...
- Criticality
 - Neutron multiplication, moderation and thermalization
 - Determination of critical configurations
 - Optimization of geometry and material composition
 - Effect of material evolution, control rods, temperature on k_{eff}
- Reaction rates
 - Fission rates and power
 - Capture rate and activation of materials
 - Detection rates

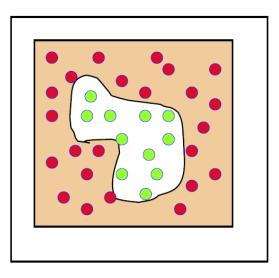
Methods of resolution

- Finite difference
- Finite elements
- Generic deterministic codes
- Monte Carlo methods

The Monte Carlo method: example of a surface calculation

It is based on solving problems by using properties of random variables and stochastic theory





Concept of neutron transport by Monte Carlo

- Neutronics of single neutrons described as particles (not fields) following the exact physics of neutrons in a medium (at least in a probabilistic sense).
- Individual, independent, random, different histories for each neutron
- Results obtained by averaging / statistical analysis of the different neutron histories

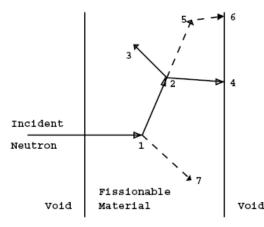
Basic processes

- Generation of neutrons from sources (position, energy, direction)
- Straight, uniform (constant speed) and free movement of neutrons between collisions
- Crossing of borders between regions with different materials, densities, temperatures, ... (geometry)
- Elastic collisions with change of direction and neutron energy moderation
- Inelastic collisions (capture, fission, (n,xn), (n,n'), ...) absorption and generation of secondary particles
- Transport of secondary particles till the end of active particles
- Recording and scoring of information for:

every collision, track segment, secondary particle creation

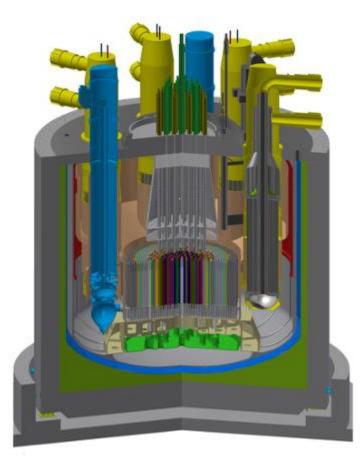
Special techniques

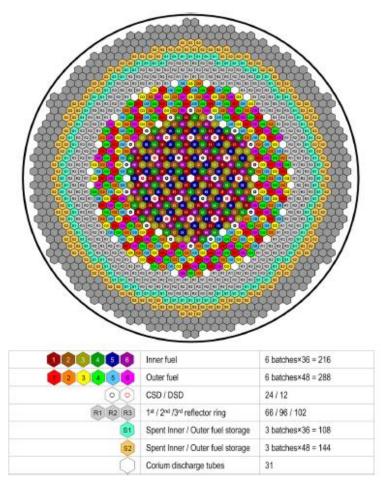
- Criticality calculations
- Variance reduction



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Practical characterization of ESFR-SMART: European SFR Safety Measures Assessment & Research Tools





Characterization of nuclear reactor core

Power map

7.4 8.2 8.3 8.2 8.4 8.3 8 8.2 7.4 8.3 6 7.6 84 84 83 8.7 84 89 87 84 83 7.3 59 857.5 83 82 81 7.7 7.8 7.9 7.9 BB 88 88 83 82 17 52 68 8.2 8.4 8.1 7.4 7.5 7.8 8 7.9 7.8 7.7 58 7.4 8.2 8.2 7.4 7.8 7.4 7.8 7.8 7.9 7.9 7.9 7.8 7.5 53 7.1 86 7.9 7.9 7.7 7.6 7.6 7.8 7.7 7.8 7.9 7.7 7.9 8.1 8.8 8 7.9 7.9 7.8 7.8 7.9 7.9 7.8 7.8 51 73 83 89 7.7 7.6 7.7 7.8 7.9 8 8 8 8 7.9 7.8 7.8 7.6 7.4 a 63 83 86 7.5 7.7 7.8 7.8 8 8 8 8 7.7 7.6 G9 82 87 7.8 7.9 7.7 7.8 7.9 7.9 8 8 7.9 7.9 7.7 7.8 7.8 7. SB 7.4 8.2 8.7 7.7 7.5 7.4 7.8 7.8 7.7 7.7 7.8 7.8 7.9 8.4 7.4 7.6 7.9 8 7.9 7.8 7.

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Main criticality safety parameters

Response	ESFR
k _{eff}	1.00148 ± 0.00008
Doppler coefficient	-215 ± 12 pcm
Coolant density coefficient	989 ± 12 pcm

2				•	•				
1 A A					, kg				
Power		BOL			EOL				
0		IF-FI	IF-FE	OF-FI	OF-FE	IF-FI	IF-FE	OF-FI	OF-FE
Δ.	U-235	5.12E+01	2.35E+01	8.65E+01	6.27E+00	1.47E+01	9.49E+00	3.52E+01	2.96E+00
	U-238	2.04E+04	9.26E+03	3.45E+04	2.47E+03	1.72E+04	8.37E+03	3.05E+04	2.28E+03
	Np-236	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.54E-04	4.36E-05	8.72E-04	7.33E-06
	Np-237	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.13E+01	1.88E+00	1.62E+01	4.29E-01
	Pu-238	1.60E+02	0.00E+00	2.71E+02	0.00E+00	8.56E+01	5.31E-01	1.69E+02	1.15E-01
	Pu-239	2.13E+03	0.00E+00	3.60E+03	0.00E+00	2.25E+03	5.60E+02	3.81E+03	1.25E+02
	Pu-240	1.33E+03	0.00E+00	2.25E+03	0.00E+00	1.34E+03	6.90E+01	2.26E+03	1.33E+01
	Pu-241	3.70E+02	0.00E+00	6.25E+02	0.00E+00	2.12E+02	4.80E+00	3.72E+02	1.07E+00
	Pu-242	4.66E+02	0.00E+00	7.88E+02	0.00E+00	3.75E+02	3.01E-01	6.74E+02	6.05E-02
	Am-241	3.50E+01	0.00E+00	5.91E+01	0.00E+00	5.13E+01	3.37E-01	1.09E+02	8.25E-02
	Am-242m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.60E+00	6.53E-03	4.44E+00	1.45E-03
	Am-243	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.82E+01	1.92E-02	9.71E+01	4.47E-03

Isotopic composition

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Uncertainty propagation in criticality safety parameters

	Response		Unc. (ESFR	%) -
	Coolant	r coefficient density ficient	5.3 ±	1.10 ⁻⁹ 7.10 ⁻⁷ 1.10 ⁻⁸
ESFR				
JEFF-3.3				
Quantity				$\Delta k_{eff}/k_{eff}$ (%)
²⁴⁰ Pu ²³⁸ U ²³⁹ Pu ²⁴⁰ Pu ²³⁸ U ²³⁹ Pu ²³⁸ U ²³⁹ Pu ²³⁸ U ²³⁸ U	(n,f) (n,n') χ (n,f) (n,n') (n,f) (n,γ) vp (n,n') (n,n') (n,r')	240Pu 238U 239Pu 240Pu 238U 239Pu 238U 239Pu 238U 238U 238U	(n,f) (n,n') χ (n,γ) (n,f) (n,f) (n,γ) v_{p} (n,γ) (n,γ)	$\begin{array}{c} 0.594 \pm 1.5 \cdot 10^{-10} \\ 0.480 \pm 3.4 \cdot 10^{-10} \\ 0.462 \pm 1.2 \cdot 10^{-9} \\ -0.417 \pm 2.5 \cdot 10^{-11} \\ -0.349 \pm 8.7 \cdot 10^{-11} \\ 0.308 \pm 2.3 \cdot 10^{-11} \\ 0.303 \pm 5.8 \cdot 10^{-12} \\ 0.294 \pm 7.2 \cdot 10^{-12} \\ 0.283 \pm 1.1 \cdot 10^{-10} \\ 0.208 \pm 1.4 \cdot 10^{-11} \end{array}$
	(n,f) rtainty in k _{ef} j		(n,γ)	$1.055 \pm 1.3 \cdot 10^{-9}$

Uncertainty propagation in isotopic composition

- Total Monte Carlo methodology
- A number of perturbed calculations are performed
- Results are obtained by statistical analysis
- Total uncertainties can be divided into decay data, cross sections and fission product yields

Uncertainty propagation in isotopic composition: actinides

lsotope	Cross sections	Fission yields	Decay data	Total
U-233	1.8	0.0	0.0	1.8
U-234	5.2	0.0	0.0	5.2
U-235	1.4	0.0	0.0	1.4
U-236	1.7	0.0	0.0	1.7
U-238	0.3	0.0	0.0	0.3
Pu-238	3.3	0.0	0.4	3.3
Pu-239	2.5	0.0	0.0	2.5
Pu-240	3.4	0.0	0.0	3.4
Pu-241	3.3	0.0	0.1	3.3
Pu-242	3.7	0.0	0.0	3.7
Am-241	3.3	0.0	0.2	3.3
Am-242m	7.0	0.0	0.3	7.0
Am-243	4.3	0.0	0.0	4.3
Cm-242	3.9	0.0	0.8	4.0
Cm-243	8.9	0.0	1.1	9.0

Uncertainty propagation in isotopic composition: fission products

lsotope	Cross sections	Fission yields	Decay data	Total
C-14	2.8	17.5	0.0	18.1
Sr-88	1.3	7.8	0.0	8.0
Sr-90	1.3	6.6	0.0	6.7
Mo-95	1.7	7.8	0.0	8.3
Tc-99	1.8	7.4	0.0	7.8
Ag-109	5.6	9.1	0.0	10.9
Ag-110m	21.3	9.5	0.0	23.5
Nd-142	5.9	7.9	0.0	10.3
Nd-143	2.0	7.1	0.0	7.3
Nd-144	1.9	6.1	0.0	6.4
Nd-148	1.8	6.2	0.0	6.6
Nd-150	1.9	9.2	0.0	9.4
Eu-151	2.6	7.1	6.5	10.0
Eu-153	6.5	4.9	0.0	8.2

Uncertainty propagation in decay heat: fission products

	Isotopic composition				Decay heat			
Isotope	Cross sections	Fission yields	Decay data	Total	Cross sections	Fission yields	Decay data	Total
C-14	2.8	17.5	0.0	18.1	2.8	17.5	0.5	18.1
Sr-88	1.3	7.8	0.0	8.0	0.0	0.0	0.0	0.0
Sr-90	1.3	6.6	0.0	6.7	1.3	6.6	0.3	6.7
Mo-95	1.7	7.8	0.0	8.3	0.0	0.0	0.0	0.0
Tc-99	1.8	7.4	0.0	7.8	1.8	7.4	3.8	8.6
Ag-109	5.6	9.1	0.0	10.9	0.0	0.0	0.0	0.0
Ag-110m	21.3	9.5	0.0	23.5	21.3	9.5	0.5	23.5
Nd-142	5.9	7.9	0.0	10.3	0.0	0.0	0.0	0.0
Nd-143	2.0	7.1	0.0	7.3	0.0	0.0	0.0	0.0
Nd-144	1.9	6.1	0.0	6.4	1.9	6.1	7.1	9.5
Nd-148	1.8	6.2	0.0	6.6	1.8	6.2	0.1	6.6
Nd-150	1.9	9.2	0.0	9.4	1.9	9.2	23.0	24.8
Eu-151	2.6	7.1	6.5	10.0	0.0	0.0	0.0	0.0
Eu-153	6.5	4.9	0.0	8.2	0.0	0.0	0.0	0.0

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Current state of nuclear data libraries allow reactor physics codes to accurately predict the behavior of nuclear reactor systems.

Huge amount of information is provided:

- Cross sections
- Decay data
- Fission neutron yield
- Fission product yields
- Uncertainties
- ...

Nuclear reactor operate safely thanks to the current level of development of nuclear data libraries.

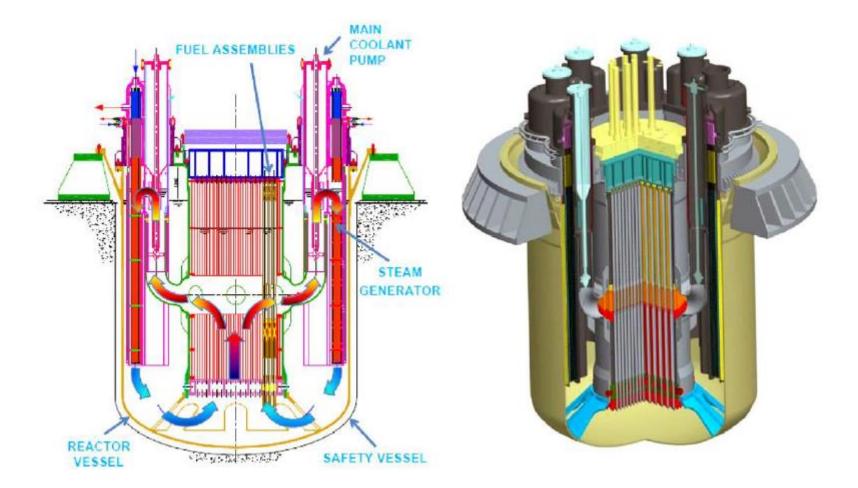
Uncertainties exist!

Uncertainty analysis can provide useful information about the status of nuclear data uncertainties, but it misses an absolute comparison.

- Target accuracies (TA) are introduced for integral parameters and for fuel cycle derived parameters.
- Defined as the maximum acceptable uncertainties for a certain reactor parameter.
- TA are defined for different isotopes, reaction, and energy regions.
- TA show the impact of the existing data uncertainties on relevant parameters.
- Used as rationale to propose a credible program of new cross section measurements.

ND strengths and weaknesses for reactor physics

ALFRED: Advanced Lead-cooled Fast Reactor Demonstrator



ND strengths and weaknesses for reactor physics

Results for target accuracies for ALFRED fast reactor:

Parameter	TA (%)	Unc. (%)
K _{eff}	0.3	0.8
$\beta_{ m eff}$	3	1.1
$\Lambda_{ m eff}$	-	20.8
Doppler coefficient (+400 K)	7	9.1
Coolant density coefficient (-5%)	7	20.3
Control rod worth	7	1.8

For fuel cycle derived parameters, target accuracy is of 20%.

- Nuclear data has a strong impact in reactor physics calculations
 - Reactor safety parameters
 - Inventory calculations
- Currently the nuclear data libraries are good enough for many applications.
- Some room for improvement has been detected.
- Ongoing effort.