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# Jubatech

# From neutronics to nuclear scenarios

# Joliot-Curie School - 2019

Nicolas Thiollière









Several countries are involved in an « energy transition »

- Low carbon emission energy sources
- Low natural resources impact
- Economic competitiveness

In this framework, nuclear industry has to face important challenges

- Ensure a very high safety level
- Find a reliable solution for nuclear wastes
- Show the feasibility of fleet dismantlement
- Produce electricity at a competitive price
- Support important required investments
- Context of high uncertainty
  - Role of anticipation
  - Scenario studies







#### Role of scenarios

Scenarios are useful tool to assess/understand complex systems

- Too much variables in interaction to build a formalized system
- Building relations in a dynamic system is a complicated
- Strong influence of human behavior or decisions (regulations, etc.)
  - Natural connexion with public/private decision making process







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- What is the role of nuclear scenario in decision process?
   Stéphanie Tillement's talk
- A fuel cycle simulation is based on operational hypothesis
  - Installations parameters (BU, cooling time, fuel fabrication time, etc.)
  - Spent fuel reprocessing strategy (LiFo, FiFo, etc.)
  - Time and duration for new technologies deployment
  - New methodology based on GSA formalism
- A fuel cycle simulation contains uncertainties that propagates
  - Nuclear data (PhD G. Krivtchik CEA, 2014)
  - Reactor simulation simplifications (PhD A. Somaini IPNO, 2017)
  - Fuel cycle simulations simplifications (FIT Project, etc.)
- Economic evaluations are built with high uncertainties
  - Individual costs dedicated to each operations
  - Calculation with the Levelized Cost of Electricity (LCOE)





#### Several scales in scenarios



# Table Of Content

Bases of Nuclear Reactor Physics
 Reactor inventory evolution
 Fuel cycle simulation and applications



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#### **1. Nuclear Reactor Physics**

- a. Basic concepts of nuclear physics
- b. Fundamentals of neutronics
- c. Neutron spectra
- d. Nuclear reactor simulation

# Reactor inventory evolution Fuel cycle simulation and applications







a. Basic concepts of nuclear physics

#### The atomic nucleus



Nuclear energy involves nucleus transformation processes

Atomic nucleus is composed by two types of nucleons

- The proton
- The neutron





Z is the atomic number
A = Z + N is the mass number
Stability depends on A and Z







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a. Basic concepts of nuclear physics

#### Valley of stability



The valley of stability is a representation of known isotopes on Z and N
Isotopes binding energy study can explain the shape of valley of stability
Binding energy is the energy required to separates a system of particles

$$-B(A, Z) = m(A, Z)c^{2} - Zm_{p}c^{2} - (A - Z)m_{n}c^{2}$$





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Liquid drop model

A simple nucleus model to explain nucleus binding energy



But with some deviations with experimental data

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a. Basic concepts of nuclear physics

# Neutron main interactions $@ 0 < E_n < 20 \text{ MeV}$







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Q is the excitation energy of the target nucleus
 Inelastic scattering is a threshold reaction

 $E_{\text{threshold}} = \frac{A+1}{A} \cdot Q$ 





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a. Basic concepts of nuclear physics

Neutron induces fission

# Laboratory United and the second second

#### Compound nucleus

#### Prompt emission

- Fission products
- Prompt neutrons (~3 / fission)
- Gamma rays
- Delayed emission
  - $-\beta^- + \bar{\nu}$
  - Delayed neutrons (~0.01 / fission)

Energy released (thermal neutron on <sup>235</sup>U)

Prompt	Energy (MeV)	Delayed	Energy (MeV)
Fission Products	169	Beta -	6.4
Neutrons	4.8	Neutrons	0.010
Gammas	7.0	Gammas	6.2
		Neutrinos	10.0
Total	180.8	Total	22.610
TOTAL		203.410	

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a. Basic concepts of nuclear physics

n,xn

# Laboratory Compound nucleus Prompt emission - 2 or more neutrons - Gamma rays $E_{\text{threshold}} = \frac{A+1}{\Delta} E_l$ (n, xn) are threshold reactions

Example

$$n + {}^{238}U \longrightarrow {}^{237}U + n' + n''$$
$${}^{237}U \longrightarrow {}^{237}Np + \beta^{-} + \bar{\nu}$$





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b. Fundamentals of neutronics

#### A nuclear reactor example



#### > Nuclear reactions are located in a small zone of the facility





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# 1. Nuclear Reactor Physicsb. Fundamentals of neutronics

#### A nuclear reactor core example





The modified fuel for use at Paks and Loviisa (Image: Rosatom)



By ORNL - originally ornl.gov now [1], Public Domain, https://commons.wikimedia.org/w/index.php?curid=2963428

Photo: Reuters







**Chain Reaction example** 

b. Fundamentals of neutronics

#### The chain reaction



For instance, a uranium-235 fission induces 2 fission products and is followed by the emission of 2 or 3 neutrons that can then hit other nucleus and so on... This is a « chain reaction".

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suite

b. Fundamentals of neutronics

#### The controlled chain reaction



If material composition is almost fixed, fission rate is constant over time





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b. Fundamentals of neutronics

#### Neutron multiplication factor









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b. Fundamentals of neutronics

## Neutron population and flux



- at a time t





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b. Fundamentals of neutronics

## Neutron population and flux

Number of neutron [-]

- with energy between E and E+dE
- in the volume dV at the position r

- at a time t

$$\blacktriangleright n(E,\vec{r},t)dEdV = \int_{\vec{\Omega}} n(E,\vec{r},\vec{\Omega},t)dEdVd\vec{\Omega}$$

Neutron flux in V = number / volume x velocity

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- Neutron flux [cm<sup>-2</sup> s<sup>-1</sup>]
  - with energy between E and E+dE
  - in the volume dV at the position r
  - at a time t

$$\varphi_{dV}(E, \vec{r}, t)dE = n(E, \vec{r}, t)dE \cdot v$$





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b. Fundamentals of neutronics

## Neutron population and flux

- Number of neutron [-]
  - with energy between E and E+dE
  - in the volume V
  - at a time t

$$\blacktriangleright N_V(E,t)dE = \int_V n(E,\vec{r},t)dEdV$$

Neutron flux in V = number / volume x velocity

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- Neutron flux [cm<sup>-2</sup> s<sup>-1</sup>]
  - with energy between E and E+dE
  - in the volume V
  - at a time t





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b. Fundamentals of neutronics

## Neutron population and flux

- Number of neutron [-]
  - with energy between E and E+dE
  - in the volume  $V_{tot}$
  - at a time t

$$\blacktriangleright N_{V_{tot}}(E,t)dE = \int_{V_{tot}} n(E,\vec{r},t)dEdV$$

Neutron flux in V = number / volume x velocity

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- Neutron flux [cm<sup>-2</sup> s<sup>-1</sup>]
  - with energy between E and E+dE
  - in the volume  $V_{tot}$
  - at a time t





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b. Fundamentals of neutronics

Neutron population and flux

- Neutron flux [cm<sup>-2</sup> s<sup>-1</sup>]
  - with energy between E and E+dE
  - in the volume  $V_{tot}$
  - for neutron with direction in  $\mbox{d}\Omega$
  - at a time t

$$\rightarrow \varphi_{V_{tot}}(E, \vec{\Omega}, t) dE d\vec{\Omega}$$

Integration over all directions

Integration over all energies

$$\blacktriangleright \varphi_{_{V_{tot}}} = \int_{E} \varphi_{_{V_{tot}}}(E) dE$$





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- Neutron flux [cm<sup>-2</sup> s<sup>-1</sup>]
  - with energy between E and E+dE
  - in the volume  $V_{tot}$
  - for neutron with direction in  $\mbox{d}\Omega$
  - for a stationary state

$$\blacktriangleright \varphi_{V_{tot}}(E, \vec{\Omega}) dE d\vec{\Omega}$$

Mono-energetic neutron beam and stationary state

Infinitely thick target so the interaction probability is very small

- A neutron can cross the target without interaction
- A neutron can undergo one unique interaction
- There is no more than one interaction per neutron

Characteristics of the experiment

- Neutron flux is  $\varphi(E)$  constrained in the surface S
- Target thickness is *dz*
- Target is composed of N nucleus per unit of volume

Number of reaction between t and t+dt in Sdz :

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 $N(t+dt) \cdot Sdz - N(t) \cdot Sdz = dN \cdot Sdz$ 







b. Fundamentals of neutronics



#### Reaction rate and cross section

- Number of target nuclides in Sdz  $N\cdot S\cdot dz$
- Neutron flux crossing the surface S  $arphi_V(E)\cdot S$
- Interaction probability on a nuclide  $\frac{\sigma(E)}{S}$ - Measurement duration dt
- Reaction rate :

 $\frac{dN}{dt} = -N \cdot \sigma(E) \cdot \varphi_V(E)$ 





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b. Fundamentals of neutronics

#### Boltzmann equation



- We consider a volume dV inside a volume V with diffusing neutrons
- The variation of the number of neutron in dV, with energy between E and E+dE, with a direction in dΩ, at a time between t and t+dt is
- [+] Ingoing neutrons in dV by diffusion during dt
- [-] Outgoing neutrons in dV by diffusion during dt
- [-] Neutron production in dE and  $d\Omega$  by scattering
- [+] Neutron disparition of dE and d $\Omega$  by any nuclear reaction
- [+] Neutron produced by fission





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b. Fundamentals of neutronics

#### Boltzmann equation

 $1 d\phi(\vec{r}, E, \vec{\Omega}, t)$ dt v  $= -div(\phi(\vec{r}, E, \vec{\Omega}, t), \vec{\Omega}) - \Sigma_{total}(r, E), \phi(\vec{r}, E, \vec{\Omega}, t)$  $+ \iint_{A^{-}} d^{2} \overrightarrow{\Omega'} \int_{0}^{\infty} dE' \Sigma(\vec{r}, E') p(E' \to E, \overrightarrow{\Omega'} \to \overrightarrow{\Omega}) \phi(\vec{r}, E', \overrightarrow{\Omega'}, t)$  $+\frac{1}{4\pi}\chi(E)\iint_{4\pi}d^{2}\overrightarrow{\Omega'}\int_{0}^{\infty}dE'\Sigma_{fiss}\left(\vec{r},E',\vec{\Omega},t\right)\cdot\phi\left(\vec{r},E',\vec{\Omega'},t\right)\cdot\nu(E')+S\left(\vec{r},E',\vec{\Omega'},t\right)$ fission neutron spectrum

Total macroscopique cross section Macroscopique fission cross section Number of neutron emitted by fission Source of neutrons

This equation cannot be directly solved for realistic systems





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c. Neutron spectra

#### Several possible spectra

#### Total neutron flux

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$$\Phi_V(t) = \int_E \varphi_V(E, t) dE$$

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- Neutron spectrum
  - Fast spectrum
  - Epi-thermal spectrum
  - Thermal spectrum



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c. Neutron spectra

#### Simple simulation

Let's try to understand simply a neutron spectrum
 MCNP simulation - PWR UOX infinite assembly



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- 96% of <sup>238</sup>U
- 4% of <sup>235</sup>U
- Coolant @ 600K - Water
- Structures @ 700KZircaloy







c. Neutron spectra

## Spectrum decomposition

## Neutron Spectrum could be divided into three parts

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- Fast spectrum

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N2P3

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- Epi-thermal spectrum
- Thermal spectrum



- In a PWR loaded with UOx, neutrons are generated by fissions
  Typical fission neutrons energy is around the MeV
- Usually, transport codes samples fission neutron energies from a Watt spectrum

$$f(E) = \frac{2\exp\left(-ab/4\right)}{\sqrt{\pi a^3 b}} \cdot \exp\left(-E/a\right) \cdot \sinh\left(\sqrt{bE}\right)$$

The Watt spectrum is not coming from theory, it's just a common function that fits well the fission neutron distribution probability





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c. Neutron spectra

#### Fast spectrum and Watt function



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c. Neutron spectra

- Once fast fission neutrons are generated, here comes the slowing-down process mainly based on elastic scattering
- Elastic scattering is considered if following conditions are respected:
  - Conservation of kinetic energy
  - Conservation of momentum
  - Conservation of the number of particles
- Elastic scattering can be considered in a classical point of view in which the neutron is a perfect rigid billiard ball
- With E in [few eV 20 MeV], energy of target is neglected







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c. Neutron spectra

#### Elastic scattering kinematics



Laboratory to center of mass frame formula
Conservation of kinetic energy and momentum in the center of mass frame

$$E_{nf} = \frac{E_{ni}}{2} \left( (1+\alpha) + (1-\alpha)\cos\theta \right) \qquad \alpha E_{ni} \le E_{nf} \le E_{ni}$$





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c. Neutron spectra

# Isotropic collision hypothesis



- Radius of the sphere is 1
- A point M is located with:
  - $\hat{\boldsymbol{\theta}}$  angle / Oz ( $\boldsymbol{\theta} \in [0, \pi]$ )
  - $\phi$  is OM projection on the plan Oxy  $(\phi \in [0, 2\pi])$
- A solid angle at M direction is defined as :  $d\Omega = \sin\theta \ d\theta \ d\phi$

Isotropic collision = 
$$P(\theta, \phi) d\Omega \propto d\Omega$$

$$\to P(\theta,\varphi)d\Omega = \frac{d\Omega}{4\pi}$$

> Oz is the particule incident direction

$$\to P(\theta)d\theta = \frac{\sin\theta}{2}d\theta$$





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c. Neutron spectra

From probability laws, we can calculate average values for energy, lethargy and angle  $\theta$  or  $\mu = \cos(\theta)$ .

$$\langle x \rangle = \int_{x_{min}}^{x_{max}} x P(x) dx$$
 with  $\int_{x_{min}}^{x_{max}} P(x) dx = 1$ 

 $\langle E_{\rm nf} \rangle = \frac{1+\alpha}{2} E_{\rm ni} \qquad \begin{cases} \mathsf{Hydrogen} & \langle E_{\rm nf} \rangle = 0.5 \ E_{\rm ni} & \mathsf{nc} \sim 20 \\ \mathsf{Carbon} & \langle E_{\rm nf} \rangle = 0.86 \ E_{\rm ni} & \mathsf{nc} \sim 80 \\ \mathsf{Sodium} & \langle E_{\rm nf} \rangle = 0.92 \ E_{\rm ni} & \mathsf{nc} \sim 120 \\ \mathsf{Lead} & \langle E_{\rm nf} \rangle = 0.99 \ E_{\rm ni} & \mathsf{nc} \sim 1600 \end{cases}$ 

The parameter  $\alpha$  is very important in the slowing down capacity of a material with mass number A





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c. Neutron spectra

Flux in hydrogen

The resolution of slowing down equation in following condition:

- Medium thermal energy is negligible compared to neutron energy
- Infinite isotropic and homogeneous medium of hydrogen
- Isotropic elastic scattering in the center of mass
- No absorption

leads to following analytic solution for the neutron flux









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c. Neutron spectra

#### Epithermal model



Physics formalism depends on neutron energy compared to target energy

- Target energy neglected : slowing down process
- Target energy non negligible : thermalization process
- A neutron population that diffuses in a medium at the temperature T can be view as a neutron gaz at equilibrium (without absorption)
- In this case, energy distribution is constant and the probability to have a neutron between E and E+dE is given by the Maxwell-Boltzmann distribution :

$$P(E)dE = \frac{2}{\sqrt{\pi}}\sqrt{\frac{E}{kT}} \cdot e^{-\frac{E}{kT}}\frac{dE}{kT}$$





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c. Neutron spectra

## Maxwell Boltzmann distribution



c. Neutron spectra

## Maxwell Boltzmann distribution



The analytic resolution of Boltzmann equation is usually not possible
 Numerical resolution from neutron transport simulation are widely used

Monte Carlo

- Based on random number samplings
- Neutrons « real » propagation simulation
- Uncertainty decreases with cpu time
- Little required simplifications
- Used as reference calculations
- MCNP, SERPENT, Tripoli, etc.

Deterministic

- Based on Boltzmann equation resolution
- Spatial simplifications
- Energy are treated as multi-group
- Resonance auto-protection
- Faster compared to Monte Carlo
- Dragon, Eranos, Apollo, etc.
- Evaluation and experimental nuclear data are fundamentals !
  - Evaluated nuclear data file are used by Monte-Carlo and deterministic codes
  - Several database are used from many countries in the world
  - ENDF, JEFF, JENDL, etc.





# **Table Of Content**

# **1. Bases of Nuclear Reactor Physics**

#### 2. Reactor inventory evolution

- a. Bateman equations
- b. Bateman solver
- c. Evolution examples
- 3. Fuel cycle simulation and applications







a. Bateman equations

The burn-up

Irradiation could be represented as a function of time or burn-up
 Burn-Up is the released energy per initial heavy mass [GWd/tHM]
 Usual burn-up is around 40 GWd/tHM (100 GWd/tHM) for a PWR (SFR)

Burn-up definition  $BU(t) = \frac{\Gamma_f \cdot t \cdot E_f}{M_{HN}}$ 

Burn-up as a function of fissioned mass  $BU(t) = \frac{N_a \cdot E_f}{A} \cdot \frac{M_f(t)}{M_{HM}}$ 

Burn-up after numerical application

Fraction in per-cent of the irradiated mass





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 $BU(t) = 9.3 \cdot 100 \frac{M_f(t)}{M_{II}}$ 

a. Bateman equations

Main form

- Bateman equations are the differential equations that describe the evolution under irradiation in a reactor core.
- It contains for each nuclide loss and creation by decay and nuclear reaction

$$\frac{dN_i}{dt} = -(\lambda_i + \sigma_i \phi)N_i + \sum_{j \neq i} (\lambda_{j \to i} + \sigma_{j \to i} \phi)N_j$$

Variation rate of the nuclide i

Loss rate by decayLoss rate by nuclear reaction

# Creation rate by decayCreation rate by nuclear reaction





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a. Bateman equations

#### Matrix form



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 $d\dot{N}$ 

dt



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N

a. Bateman equations

#### Mean cross section

Reaction rate defined in Bateman equations:

$$N\sigma\phi = \int N\sigma(E)\varphi(E)dE$$
Normalized flux in E and E+dE
$$=> [cm^{-2} \cdot s^{-1} \cdot MeV^{-1}]$$

Mean cross section simplifications

$$N\sigma\phi=N\langle\sigma
angle\phi$$
 with

A mean cross section aggregates the cross section in a unique number

The total flux is then used to normalize

$$\begin{split} \langle \sigma \rangle &= \frac{\int \sigma(E) \varphi(E) dE}{\int \varphi(E) dE} \\ \phi &= \int \varphi(E) dE \end{split}$$

Total flux in the system =>  $[cm^{-2} \cdot s^{-1}]$ 





a. Bateman equations

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#### Mean cross section



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a. Bateman equations

Reaction rate vs mean XS

In practice, it is possible to calculate

Reaction rates

- Reaction rates are calculated at each steps of the transport code calculation as the multiplication of the flux and cross sections.
- Number of reaction rate to calculate
   Number of isotopes x Number of reactions

#### Mean cross sections

- Mean cross sections are calculated at the end of the transport calculation

One observable to asses
 Neutron flux



A very high precision is required
 More than 10 000 energy groups

For a complex calculation inducing a high number of isotopes, mean cross sections based evolution decrease the CPU time by a factor ~30 (SMURE team)





a. Bateman equations

Normalization

Neutron spectrum is included inside mean cross sections
 Bateman equation depends on neutron total flux

$$\frac{dN_i}{dt} = -(\lambda_i + \langle \sigma_i \rangle \phi)N_i + \sum_{j \neq i} (\lambda_{j \to i} + \langle \sigma_{j \to i} \rangle \phi)N_j$$

- Neutron flux in a reactor is not precisely known and depends on:
  - Thermal power of the reactor core
  - Burn-up of the fuel
  - Control rod position
  - Neutronic poisons amount (boron, Gd, etc.)
  - etc.

In practice, user calculates/imposes the neutron flux according to the power





a. Bateman equations

## Normalization

# A simple solution could be to consider a constant flux during irradiation

Target irradiation by neutrons



- Possible experimental flux : 10<sup>6</sup> cm<sup>-2</sup> s<sup>-1</sup>
- Number of atoms in the target : 10<sup>24</sup>
- ▶ Reaction rate : 10<sup>6</sup> absorption s<sup>-1</sup>
- ▶ Irradiation time : 10<sup>5</sup> s
  - Composition modification is small
  - Spectrum modification is small
  - Neutron Flux is stationary

Nuclear power plant core irradiation



- Possible experimental flux : 10<sup>14</sup> cm<sup>-2</sup> s<sup>-1</sup>
- Number of atoms in the target : 10<sup>29</sup>
- Reaction rate : 10<sup>20</sup> absorption s<sup>-1</sup>
- Irradiation time : 10<sup>8</sup> s
  - Composition modification is significant
  - Spectrum modification is significant
  - Neutron Flux is not constant
- Flux normalization is possible for experiments with low neutron flux
  For a reactor evolution, the flux can't be considered as constant





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a. Bateman equations

Neutron flux evolution

Infinite assembly PWR simulation with SMURE - UOx (3.7% <sup>235</sup>U)
 Constant thermal power during irradiation



During irradiation, some neutron absorbent are generated
Neutron flux increase in order to have a constant thermal power





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a. Bateman equations

N2P3

## Spectra evolution



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a. Bateman equations

Mean XS evolution

Mean cross sections are strongly impacted during the burnup



a. Bateman equations

In practise

During neutron irradiation, a lot of parameters are evolving

- Neutron spectrum and neutron total flux
- Mean cross sections

Neutronic data need to be updated a lot of time to avoid biases

- Coupled transport calculation / evolution calculation
- Compromise between calculation time and required precision







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a. Bateman equations

Energy released by fission

Thermal power and neutron flux relation is given by:

$$P_{th} = \sum_{i} N_i \int \sigma_i^{fis}(E) \phi(E) \epsilon_i(E) dE$$

- N<sub>i</sub> is the number of fissile nucleus
- $\sigma_i$  is the cross section of nucleus i
- $\Phi$  is the neutron flux
- $\epsilon_i$  is energy released by the nucleus i

#### Energy released by a fission on <sup>235</sup>U by a thermal neutron

Prompt	Energy (MeV)	Delayed	Energy (MeV)
Fission Products	169	Beta -	6.4
Neutrons	4.8	Neutrons	0.010
Gammas	7.0	Gammas	6.2
		Neutrinos	10.0
Total	180.8	Total	22.610
TOTAL		203.410	





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2. Reactor inventory evolution Resolution b. Bateman solver simple example Simple method but not really used  $\frac{dN_x}{dt} = -\lambda_x N_x(t)$  $N_x(0) = N_0$ - Not precise - Not stable System to be solved:  $y = N_x$  $\frac{dy}{dt} = f(y,t) \qquad y(0) = y_0$  $f(y,t) = -\lambda_x N_x(t)$ Time discretization and first order development:  $y(t_i + \Delta t) = y(t_i) + \Delta t \left(\frac{dy}{dt}\right)_{t} + O(\Delta t^2)$ 

 $y_{i+1} = y_i + \Delta t f(y_i, t_i) + O(\Delta t^2)$ 





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b. Bateman solver

Resolution



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b. Bateman solver

Runge-Kutta

- Runge-Kutta methods are widely used to solve evolution equations
  Advantages:
  - Easy to program and to use
  - Usually stable
  - Easy to modify the time binning
  - Initial conditions allows integration
- Drawbacks:
  - High calculation time

Runge-Kutta 2



$$\rightarrow y_{i+1} = y_i + \Delta t r_2$$

Runge-Kutta 4  $r_{1i} = f(y_i, t_i)$   $r_{2i} = f(y_i + \frac{\Delta t}{2}r_{1i}, t_i + \frac{\Delta t}{2})$   $r_{3i} = f(y_i + \frac{\Delta t}{2}r_{2i}, t_i + \frac{\Delta t}{2})$   $r_{4i} = f(y_i + \Delta t r_{3i}, t_i + \Delta t)$ 

→ 
$$y_{i+1} = y_i + \frac{\Delta t}{6} (r_{1i} + 2r_{2i} + 2r_{3i} + r_{4i})$$





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c. Evolution examples







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c. Evolution examples

Example - PWR UOx







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c. Evolution examples

Example - PWR UOx



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c. Evolution examples







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d. Reactor evolution biases

# Scheme calculation

 Numerical resolution of a full core calculation is usually not possible because the calculation time is too high (deterministic or Monte-Carlo)
 In practice, a full core calculation is divided in two steps

- Cell calculation
  - Stationary Boltzmann equation with no leakage
  - Energy condensation and space homogenization
  - => XS multigroup
- Core calculation
  - Diffusion equation

$$-D\Delta\Phi = \nu\Sigma_f\Phi - \Sigma_a\Phi$$







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# **Table Of Content**

# Bases of Nuclear Reactor Physics Reactor inventory evolution

## 3. Fuel cycle simulation and applications

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- d. MOx strategy impact
- e. Plutonium multi-recycling in PWR



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### **3. Fuel cycle simulation / applications**

#### a. The fuel cycle simulator

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#### The fuel cycle



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A lot of fuel cycle simulators are developed worldwide

- COSI
  - Developed by CEA since 80's to support french nuclear fleet management
  - Very detailed simulating framework with a lot of derived data
- CLASS (Core Library for Advanced Scenario Simulation)
  - Developed by CNRS since 2010
  - Flexible C++ library connected to ROOT analysis framework
  - Used by IRSN for ASTRID scenario calculations
- CYCLUS
  - Developed mainly by university of Madison-Wisconsin since few years
  - Agent-based fuel cycle simulator based on a powerful dynamic resource exchange solver
- ORION (National Nuclear Laboratory, UK)
- DYMOND (Argonne National Lab, US)
- DANESS (Private company Nuclear-21)
- Etc.





## **3. Fuel cycle simulation / applications**

#### a. The fuel cycle simulator

#### The code CLASS


Most important developments are related to physics models for reactors

- Fuel Loading Model (FLM)
  - Neutronic data predictor
  - Fresh fuel loading algorithms
- Cross Section Predictor (CSP)
- Bateman Solver (BS)

> Up to now, several reactors have been implemented in CLASS

- Pressurized Water Reactors
  - ➡ UOx
  - ➡ MOx
  - → MOx-Am
  - MOx on enriched uranium support
- Sodium fast reactors
  - ➡ ESFR
  - ➡ ASTRID







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a. The fuel cycle simulator

## An example of FLM

# Choice of the spatial scale

- Pin
- Assembly
- Full core



# Choice of the transport code

- Monte Carlo
  - Serpent
  - → <u>MĊNP / SMURE</u>
- Deterministic
  - Donjon/Dragon
  - ⇒ etc.

## Choice of the Pu vector boundaries



# Sampling on LHS with sum = 1 Run of thousands simulations

F. Courtin, et al. Neutronic predictors for PWR fuelled with multi-recycled plutonium and applications with the fuel cycle simulation tool CLASS, Progress in Nuclear Energy, Volume 100, 2017.





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a. The fuel cycle simulator

# An example of FLM

# Prediction of reactivity evolution

- Polynoms
- <u>Neural networks</u>

F. Courtin, et al. Neutronic predictors for PWR fuelled with multirecycled plutonium and applications with the fuel cycle simulation tool CLASS, Progress in Nuclear Energy, Volume 100, 2017.







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a. The fuel cycle simulator

Precision of the predictor

Precision of prediction from an independent set of data

- 100 independant runs
- Represented points are relative deviation mean values
- Error bars are standard deviations



# An artefact at small irradiation time is coming from xenon effect

Fanny Courtin. Etude de l'incinération du plutonium en REP MOX sur support d'uranium enrichi avec le code de simulation dynamique du cycle CLASS. Physique Nucléaire Expérimentale [nucl-ex]. Ecole nationale supérieure Mines-Télécom Atlantique, 2017. Français. NNT : 2017IMTA0044 . tel- 01668610







a. The fuel cycle simulator

## Fuel batching



**Fig. 2.**  $k_{\infty}^{frac}$ ,  $k_{\infty}$  and  $k_{threshold}$  of a PWR MOX with a maximum burnup achievable of 35 GWd/tHM and a 3 batches management.

Baptiste Leniau et al. A neural network approach for burn-up calculation and its application to the dynamic fuel cycle code CLASS.





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#### Maximal burn-up

# a. The fuel cycle simulator







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a. The fuel cycle simulator

# An example of XSM

#### Prediction of cross sections

- Polynoms
- This example : Neural networks

Fanny Courtin. Etude de l'incinération du plutonium en REP MOX sur support d'uranium enrichi avec le code de simulation dynamique du cycle CLASS. Physique Nucléaire Expérimentale [nucl-ex]. Ecole nationale supérieure Mines-Télécom Atlantique, 2017. Français. NNT : 2017IMTA0044 . tel-01668610







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# **3. Fuel cycle simulation / applications** a. The fuel cycle simulator

#### Precision of (n,f)



Fanny Courtin. Etude de l'incinération du plutonium en REP MOX sur support d'uranium enrichi avec le code de simulation dynamique du cycle CLASS. Physique Nucléaire Expérimentale [nucl-ex]. Ecole nationale supérieure Mines-Télécom Atlantique, 2017. Français. NNT : 2017/MTA0044 . tel- 01668610

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Precision of (n,g)

a. The fuel cycle simulator



Fanny Courtin. Etude de l'incinération du plutonium en REP MOX sur support d'uranium enrichi avec le code de simulation dynamique du cycle CLASS. Physique Nucléaire Expérimentale [nucl-ex]. Ecole nationale supérieure Mines-Télécom Atlantique, 2017. Français. NNT : 2017/MTA0044 . tel- 01668610

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Precision of (n,2n)

a. The fuel cycle simulator



Fanny Courtin. Etude de l'incinération du plutonium en REP MOX sur support d'uranium enrichi avec le code de simulation dynamique du cycle CLASS. Physique Nucléaire Expérimentale [nucl-ex]. Ecole nationale supérieure Mines-Télécom Atlantique, 2017. Français. NNT : 2017/MTA0044 . tel- 01668610

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a. The fuel cycle simulator

## Precision of evolution calculation







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Fanny Courtin PhD. IMT Atlantique 2017.

# Fuel Cycle Simulators (FCS) are developed for many purposes

- Study existing nuclear fleet in support for industrial operation optimization
- Study and analysis of electro-nuclear future trajectories for prospective reflexions
- Verification and/or assessment of nuclear fleets by safety authorities
- Training and educational tool for the fuel cycle understanding

# FCS confidence outputs is a major issue

# FCS bias & uncertainty

- Reactor simplifications
  - System simulations
  - Nuclear Data
- Scenario simplifications
  - Technical parameters
  - Facility operating hypothesis
- FCS use
  - Problem definition
  - Problem solving method





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Reactors studies

- Code development and qualification
- Benchmarks
- Precise reactor coupling with FCS
- Fuel cycle studies
  - Functionality testing
  - Global benchmarks
- FCS use
  - Sociology related question

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Scenarios methodology

## Historical methodology to build and run nuclear scenario



Fanny Courtin PhD. IMT Atlantique 2017.

Scenarios methodology

New methodology is used to define reference scenarios



b. Uncertainty and bias

#### Nuclear data

enrichment

- A fuel cycle simulator is using nuclear data for physics models :
  - Fuel loading models
  - Irradiation in reactors
  - Cooling in facilities



natural uranium

Figure 6.20: Scenario C: fuel cycle between 2038 and 2100

G. Krivtchik. PhD, CEA 2014.

reprocessed





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For all simulations, nuclear data are sampled with the correlations



Nuclear data have a significant impact on Pu and MA inventories
But the effect is probably small compared to other uncertainty sources

G. Krivtchik. PhD, CEA 2014.





A fuel cycle simulator is using neutronic predictors from reactor simulations



Reactor simulations are very simplified

- Full core calculation scheme is complex
- A lot of calculation are required
  - Use of infinite assembly calculation

# Impact on neutrons axial leakage



A. Somaini. PhD, IPNO. 2017





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A fuel cycle simulator is using neutronic predictors from reactor simulations

Infinite assembly

- Impact of the assembly cross-talk



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> A fuel cycle simulator is using neutronic predictors from reactor simulations

Core coupling with scenario calculation

100

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- Transport code : Dragon
- Core calculation : Donjon
- Cycle calculation : CLASS



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b. Uncertainty and bias

Lot of uncertainties

Fanny Courtin PhD. IMT Atlantique 2017.

- A complex nuclear fleet is composed by many reactors in interaction
  - Very detailed fleet
    - VS
  - Few macro reactors



For a complex french nuclear fleet simulation, detailed fleet has a similar behavior when compared to macro reactors fleet.
Except for some scenarios which is explained by a lack of plutonium





From neutronics to nuclear scenarios Nicolas Thiollière - IMT Atlantique A fuel cycle code functionality is the translation into computer software language of a physical or technical process related to nuclear facilities.

Reference	Functionality to develop	
At each reactor loading, the reactor	At each reactor loading, the reactor	
fresh fuel composition is constant	fresh fuel composition depends on avail-	
	able material isotopic composition	
The reactor load factor is constant over	The reactor load factor takes into	
the reactor lifetime	account precise industrial constraints,	
	such as partial refueling	Fresh fuel @ B.O.C.
The mean cross sections used to perform	The mean cross sections used to perform	
the fuel evolution in reactor are calcu-	the fuel evolution in reactor are updated	FE (Fixed Fraction)
lated at BOC and kept constant during	according to fuel composition	- Fissile fraction is constant
the cycle		
The reactor first cycles composition is	The exact reactor first cycles composi-	FLM (Fuel Loading Model)
not taken into account and is assumed	tion is used	- Reactor requirements
to be the steady states composition		- Available isotopes stock

Table 1: Examples of simplified and more complex functionalities.

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b. Uncertainty and bias

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#### c. The french fleet simulation

## The PRIS Database







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#### c. The french fleet simulation

## The PRIS Database

France	•						<u> </u>
			SU	JMMARY			_
Nuclear Power React	ors				Electricity Product	ion Share in 2018	Tr
Under Construction	Operationa	I	Long-Term Shutdown	Permanent Shutdown			
1	58		0	12		Nuclear	Share [%]
						Non Nuc	lear Share [
Annual Electrical Po	wer Production				28.33 5	%	
Total Electricity Produc	Total Electricity Production (including Nuclear)			ction	71.67 %		
548600.00 G	548600.00 GW.h			00 GW.h			
(Net, 2018)			(Net, 2018)				
			RE	ACTORS			
					Reference	Gross	Firet
Name	*	Туре	Status	Location	Unit Power	Capacity	Conne
		-			[]	[MW]	
BELLEVILLE-1		PWR	Operational	LERE	1310	1363	1987
BELLEVILLE-2		PWR	Operational	LERE	1310	1363	1988
BLAYAIS-1		PWR	Operational	BRAUD ST.LOUIS	910	951	1981
BLAYAIS-2		PWR	Operational	BRAUD ST.LOUIS	910	951	1982
BI AVAIS-3		PWR	Operational		010	051	1083
					310	331	1000
BLAYAIS-4		PWR	Operational	BRAUD STLOUIS	910	951	198





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#### c. The french fleet simulation

## The PRIS Database

Reactor Type <b>PWR</b>	Model CP1	Owner ELECTRICITE DE FRANCE	Operator ELECTRICITE DE FRANCE
Reference Unit Power (Net Capacity) 910 MW <sub>e</sub>	Design Net Capacity 910 MW <sub>e</sub>	Gross Capacity 951 MW <sub>e</sub>	Thermal Capacity 2785 MWt
Construction Start Date 01 Jan, 1977	First Criticality Date <b>20 May, 1981</b>		
First Grid Connection 12 Jun, 1981	Commercial Operation Date 01 Dec, 1981		

		LIFETIME PERFORMANCI	E	
Electricity Supplied 215.97 TW.h	Energy Availability Factor <b>76.6 %</b>	Operation Factor <b>77.9 %</b>	Energy Unavailability Factor 23.4 %	Load Factor 72.7 %
Lifetime performance calc	ulated up to year 2018			

			OPER	ATING HISTORY				
Year Electricity Supplied [GW.h]	Electricity Supplied	Reference Unit Power	Annual Time On Line	Operation Factor	Energy Availability Factor [%]		Load Factor [%]	
	[MW] [***	[70]	Annual	Cumulative	Annual	Cumulative		
1981	1636.200	920	2584	70.2	65.6	65.6	65.6	65.6
1982	6129.800	910	7588	86.6	81.5	80.2	76.9	76.0
1983	3453.000	910	4285	48.9	43.9	62.8	43.3	60.3





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c. The french fleet simulation

# French fleet history

# Goals

- Centralize available data
- Get the initial conditions
- Compare with available data

- Lack of data
  - Reactor deployment
  - First loadings
  - Discharge burn-up
  - Fuel management strategy





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French fleet schematic view with two fuel management stages

- The UOX level
- The MOX level
- Nuclear waste

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## Plutonium inventory



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## Pu stocks and pools



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## Minor Actinides inventory



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Comparison with Americium

- ▶ <sup>241</sup>Am production is smaller than <sup>237</sup>Np production in reactor
  - <sup>241</sup>Am is mainly produced outside from the reactor by <sup>241</sup>Pu decay
  - <sup>241</sup>Am increases during fuel cycle evolution

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Reactor



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Radiotoxicity of total inventory @ 2015



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<b>B. Fuel cycle simulation / applications</b> d. MOx strategy impact	Nide Sweeping N	⁄lethodo	logy
	Input Data	Min. Value	Max. Value
Global sensitivity analyse framework	PWR-UOx BU [GWd/t]	30	60
- Wide design of experiment	PWR-MOx BU [GWd/t]	30	60
- High number of simulations	<b>PWR-MOx Fraction</b>	0	0.20
- Macio reactors simulation	Pool Cooling time (y)	0	20
	Stock Management	FiFo /	/ LiFo
Stock Infinite Unat U	Spent Pool - UO	,	
Stock with Pu Pu Pu PWR - MOx	Spent Pool - MOx	:	Stock Spent MOX
Stock Infinite Udep	ation		Waste

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## **3. Fuel cycle simulation / applications** d. MOx strategy impact

Data storage



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d. MOx strategy impact

### Plutonium inventory @ EOS

Total plutonium production





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d. MOx strategy impact

N2P3

Pu production is not linear with PWR UOX burn-up

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- High for small irradiation time
- Smaller for high burn-up
- > Pu production rate is higher for small PWR UOX burn-up



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## **3. Fuel cycle simulation / applications** d. MOx strategy impact

## Plutonium equilibrium



- Neptunium production mainly depends on two variables
  - Production increases with PWR-UOx burn-up
  - Production decreases with PWR-MOx fraction







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d. MOx strategy impact

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Neptunium production

$$^{235}U(n,\gamma) \rightarrow ^{236}U(n,\gamma) \rightarrow ^{237}U \xrightarrow{}_{6.7d} ^{237}Np$$
ways
$$^{238}U(n,2n) \rightarrow ^{237}U \xrightarrow{}_{6.7d} ^{237}Np$$
wreases with BU

2 production pathw Production rate increases with BU



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d. MOx strategy impact

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## MOx / UOx comparison



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Joliot-Curie School, Saint Pierre d'Oléron, France September 22-27, 2019 French « official » nuclear scenarios were since the 80's very clear

- Nuclear production was supposed to be constant during the century
- Sodium fast reactors will be deployed to manage Pu and MA







e. Pu multirecycling in PWR

#### Design Of Experiment



e. Pu multirecycling in PWR

Some results



Reference scenarios built with detailed fleet from GSA and macro reactors

- are keeping the stabilization properties of Pu and MA,
- are allowing to better quantify trajectories.





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