Numerical models for nuclear reactor physics

Towards a common framework

From GT11 prospective's contribution :

LPSC - Grenoble

A. Bidaud, A. Billebaud, N. Capellan, S. Chabod, V.Ghetta, A. Nuttin, P. Rubiolo

LPC – Caen

J. –L. Lecouey, F.-R. Lecolley, N. Marie

SUBATECH - Nantes

L. Giot, N. Thiollière

IJC Lab - Orsay

X. Doligez, M.Ernoult

Introduction : a little flashback

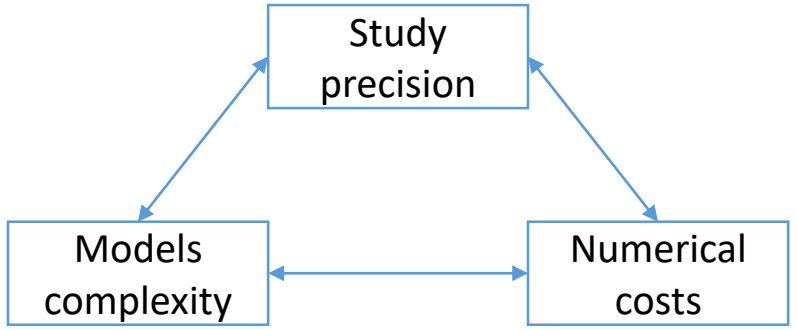
- Research motivated for exploring nuclear systems potentialities for future nuclear energy *(wastes production and natural resource consumption)*
  - ~1996 first recycling studies (ADS & MSR)
  - ~2003 Beginning of MURE (MCNP Utility for Reactor Evolution)
  - Since then numerous studies involving diverse systems (CANDU, REP, RNR) – comparison between thorium and uranium fuel cycles

Pros and cons of different reactor and fuel technologies
Building a know-how in reactor modeling
Fuel the societal debate in the frame of the French law (Loi "Bataille" – 1991)

- Numerous systems studied as a way to explore reactor model options.
  - Continuous improvement of modeling tools since 2003

→ Slow evolution towards the tough spots in reactor modeling – more fundamental positioning on neutron behavior in critical media

- IN2P3 research actions : twin track approach
  1. ***Study of systems of interest*** (for the French fleet in the short term : SMR and EPR)
     « cycle » and « transient » studies
  2. **Control and reduction of uncertainties → Modeling effort**
     Numerical biases, Nuclear Data, Operational data,…



Presentation outline :

- Boltzmann's equation
  - Principle and numerical difficulties
  - A two level calculation scheme for thermal neutron systems
  - Different limitations and improvement propositions
  - Nuclear data uncertainties

- Coupled calculations
  - Fuel evolution
  - Reactor models for fuel cycle simulations
  - Thermal-hydraulics coupling
  - Uncertainty propagation

- Towards a common numerical framework to gather all models
  - Interest and challenges
  - Some key points
  - As a first step : the OSCAR project

Criticality calculations : solving Boltzmann's equation

- Boltzmann's equation : looking for $\psi(\vec{r}, \hat{\Omega}, E, t)$

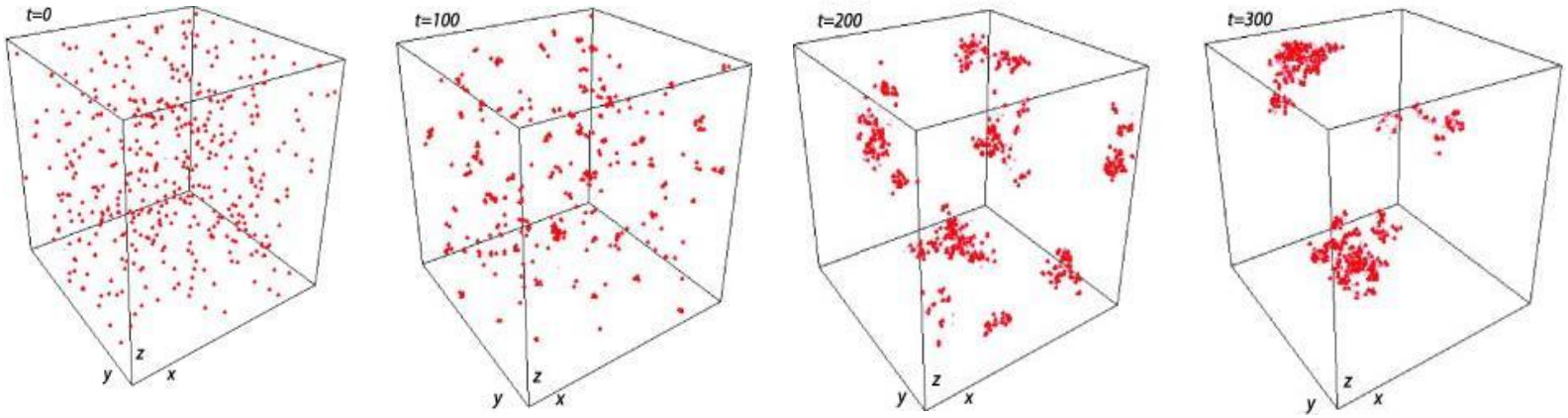
$$\frac{1}{v}\frac{d\psi}{dt} = -\hat{\Omega}.\nabla\psi - \Sigma_{tot}\psi + \int_{E'=0}^{\infty}\int_{4\pi}\Sigma_S(E' \to E, \hat{\Omega}' \to \hat{\Omega})\psi\, dE' d\hat{\Omega}' + \frac{\chi}{4\pi}\int_{E'=0}^{\infty}\int_{4\pi}\nu\Sigma_f\psi\, dE' d\hat{\Omega}' + S$$

→ *Temporal variation = - Disappearance by leakage and by collision + Production by transport, fission and external sources*

- k_{eff} definition for the stationary equation : $\boldsymbol{M}\phi = \frac{1}{k_{eff}}\boldsymbol{F}\phi$ → Transient studies often consider criticality → $\Phi(\vec{r}, E, t, ..) = N(t).\phi(\vec{r}, E, ...)$

- Deterministic methods
  - → Energy, space and angle binning
  - → Impossible to compute on a full scale reactor

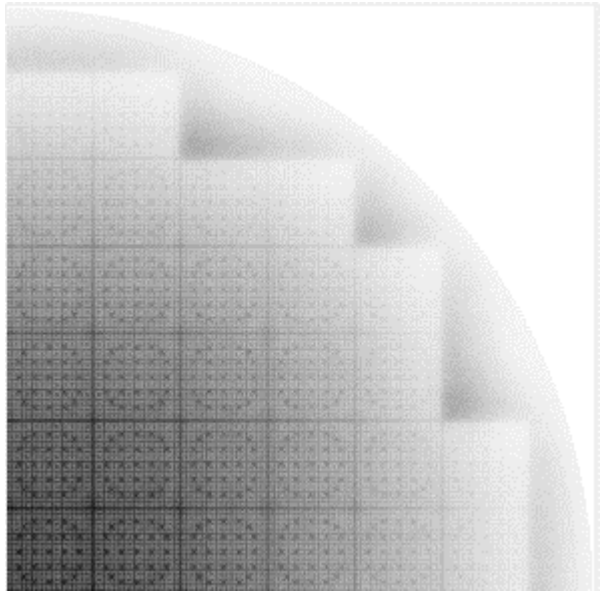
E. Dumonteil, F. Malvagi, A. Zoia et al., Annals of Nuclear Energy, vol. 64, p. 612-618, 2014



- Monte-Carlo methods
  - → Simulation of a great number of neutron history
  - → Story begins at the end of a previous one
  - → Source convergence issues (for thermal reactors)

Solving the neutron transport equation is "impossible" on large reactor with a thermal spectrum

Solving Boltzmann's equation : a two step algorithm for thermal reactors



Mean behavior of each assembly :

→ 2 energy groups

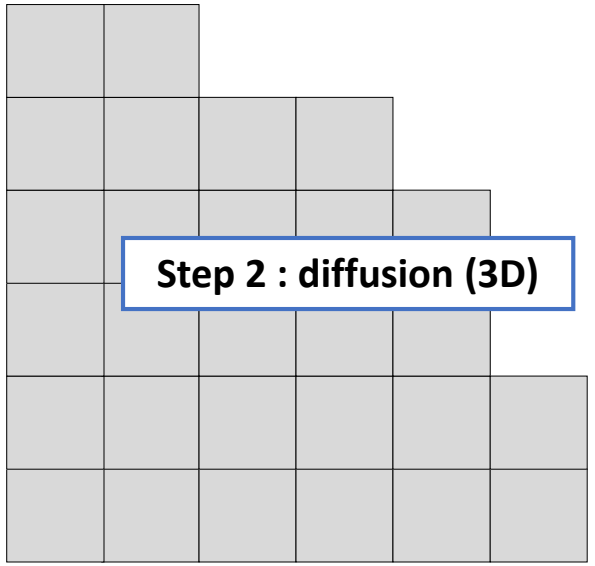
→ Homogenized geometry

→ No more angle variable (Fick's law)

Extreme simplification of the neutron balance

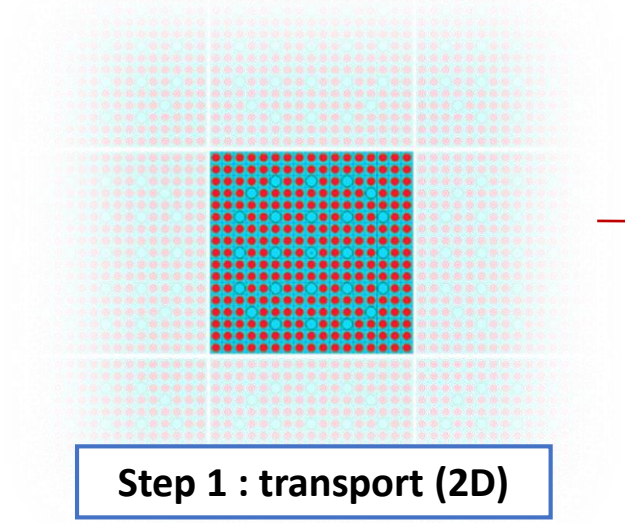
$$\Delta\phi + \frac{\nu\Sigma_f - \Sigma_a}{D}\phi = 0$$

$$\Sigma_i = N.\frac{\int_0^{E_c} \sigma_i(E)\phi(E)dE}{\int_0^{E_c} \phi(E)dE}$$

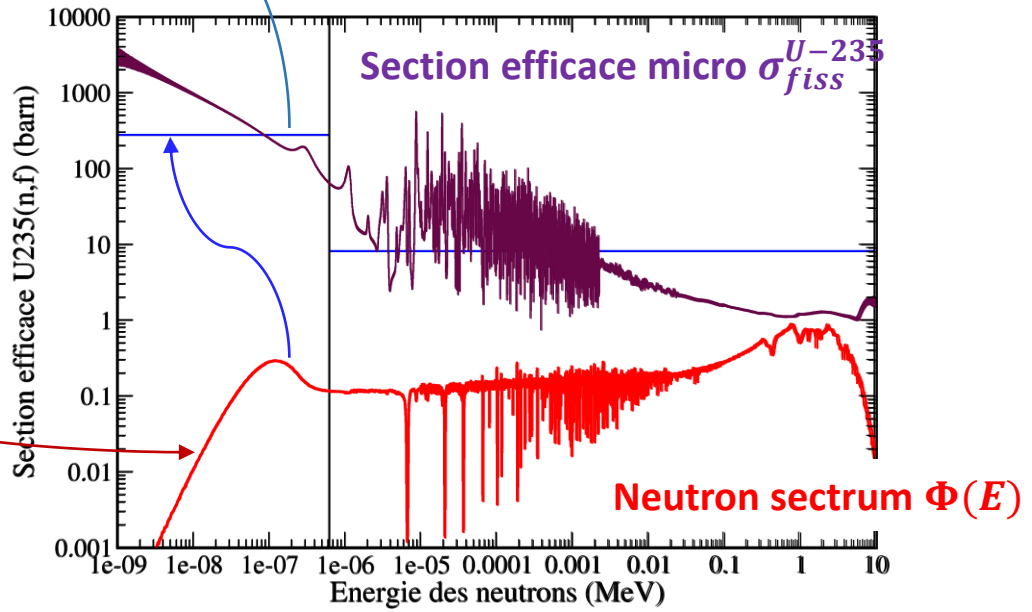


Step 2 : diffusion (3D)

➢ Precise resolution of the transport equation on limited geometry, with periodic boundaries



Step 1 : transport (2D)



Diffusion approximation : an efficient method with strong limitations

Limitation #1 – Transport calculations are performed on an infinite geometry :

- → Diffusion data do not depend on the localization
- → Environment is completely neglected

➢ Issues for interfaces modeling :

A strong increase of the neutron flux at the interface due to the local increase of fission cross section

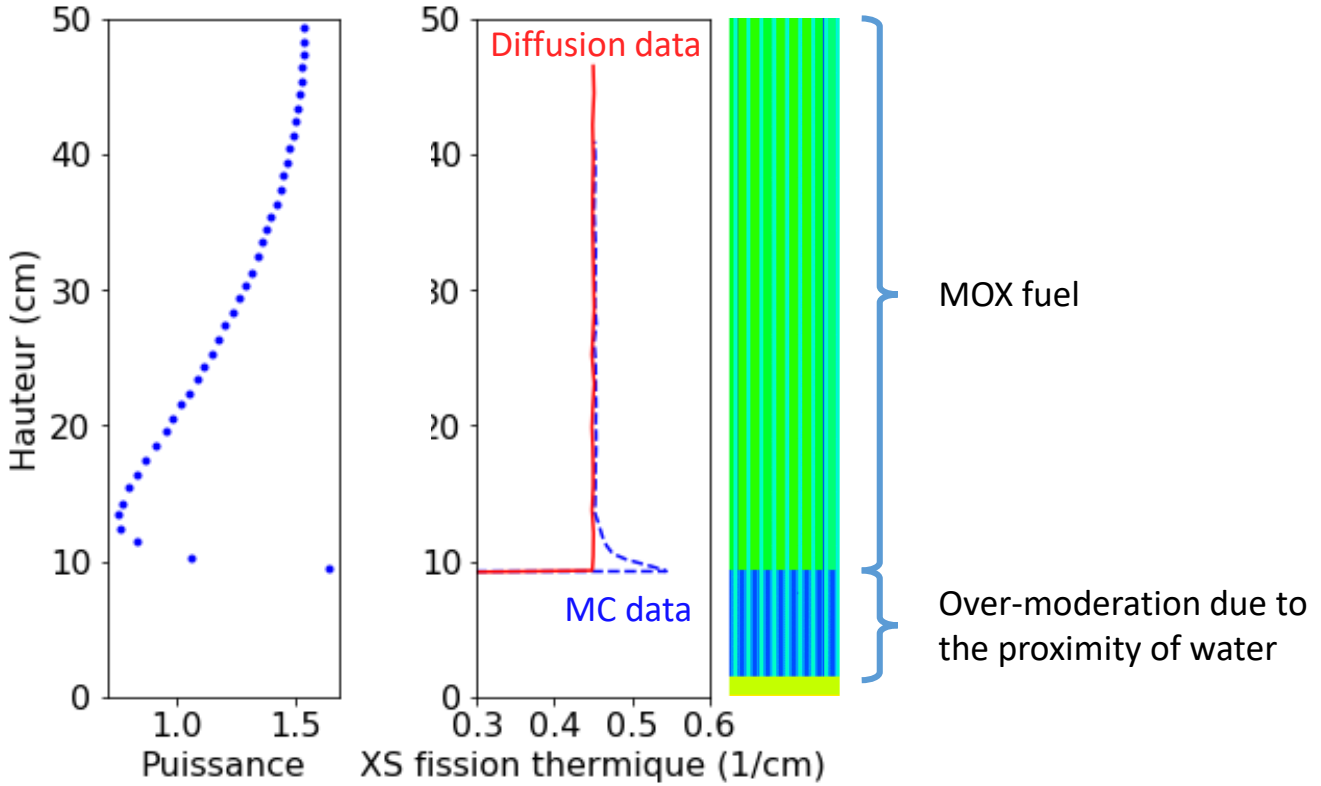
→ Badly modeled by the classical transport/diffusion scheme

➢ Improve the production/handling of diffusion data

- → New variable (localization, neighbors, boron,…)
- → New interpolation methods (ANN,…)

→ *NEEDS project (IN2P3/IRSN/Poly Montreal) : MADIFF*

→ *Collaboration with Framatome : Adien Rispo PhD thesis*



Limitation #2 – How to calculate diffusion data for reflectors ?

Without fissile material, the solution of transport equation is 0

→ *Data in the reflector depends on the fuel composition… but the fuel behavior depends on the reflector properties*

Limitation #3 – The system is supposed to be critical

→ Use of the α −mode decomposition

Uncertainties induced by nuclear data : propagation studies

➢ Numerical biases have to be compared to other sources of errors, specially uncertainty induced by nuclear data

Total-Monte Carlo

➢ Principle :

Creation of *n* different nuclear data file *TENDL*

↓

n evaluations (for one given nucleus)

↓

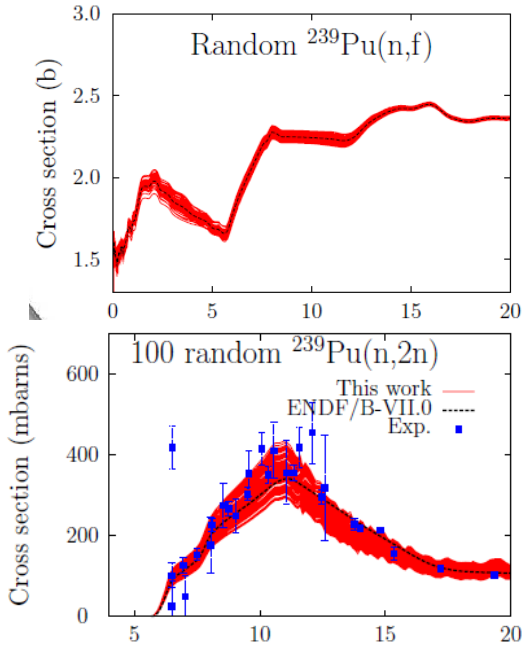
n criticality MC calculations

↓

$\overline{k_{eff}}$; $var(k_{eff})$

For each studied nucleus

D. Rochman et al.



Generalized perturbation theory (GPT)

➢ The variance of a given observable is related to the sensitivity coefficients and the covariance matrix of the parameters

$$var(k_{eff}) = S_\sigma^t . cov(\sigma_i, \sigma_j) . S_\sigma \qquad S_\sigma^k = \frac{\delta k / k}{\delta \sigma / \sigma}$$

➢ The adjoint equation allows sensitivity calculations

$$\frac{1}{k_{eff}} \boldsymbol{F}^+ \phi^+ = \boldsymbol{M}^+ \phi^+ \longrightarrow S = \frac{\left\langle \phi^+ \left| \left(\frac{\partial \boldsymbol{M}}{\partial \sigma} - \lambda \frac{\partial \boldsymbol{F}}{\partial \sigma} \right) . \phi \right. \right\rangle}{\langle \phi^+ | \boldsymbol{F} \phi \rangle}$$

➢ A single direct calculation and an adjoint calculation are sufficient to estimate the uncertainties (once the covariance matrix determined)

→ Easily accessible by deterministic methods

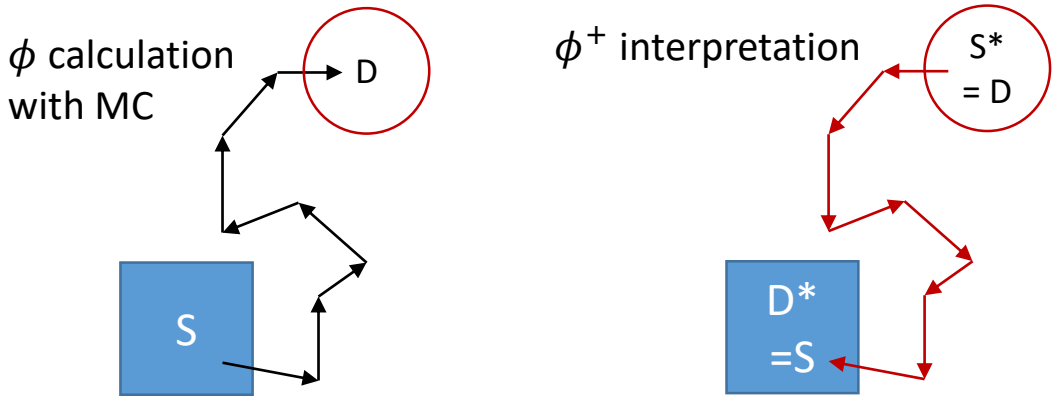
➢ TMC : high computational costs + difficult physical interpretation BUT exact calculations

➢ GPT : more physical information and reasonable computational needs BUT approximate methods and needs of a covariance matrix

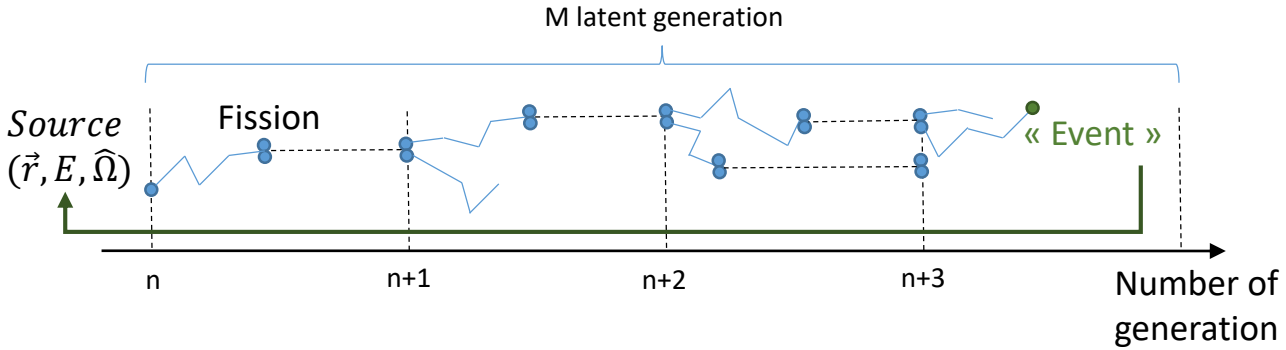
→ Explore both methods and their complementarity – production of covariance with TENDL (*Thèse Eliot Party – 2019)*

Sensitivity calculations : the revenge of Monte-Carlo methods in mid 2010s

- Physical interpretation of the adjoint flux : its relative importance related to a detection
  → « Going back in time »



- Recording successive neutron generation to track the history of fission chains
- The importance of a source neutron is then measured on every observable calculated by MC methods



- Number of *LatGen* to be adjusted regarding the observable (power distribution needs more than 100 latent generations)

Pamela Lopez et al. (2021)

- Number of LatGen directly linked to the memory needs

→ Sensibility to double differential cross-section, resonance parameters, temperature distribution,…
→ Sensitivity of modal decomposition
→ *NEEDS project (IN2P3/IRSN/CEA) : SUDEC*

Outline :

- Some take home messages :
  - → Two step calculation scheme is mandatory for large scale reactors
  - → Homogeneous data production is a key issue :
    - MC methods may improve their relevance
    - Modal decomposition removes the assumption of stationarity
  - → MC methods have shown great potentialities for sensitivity calculations

MC/Diffusion coupling calculation scheme

- Boltzmann's equation
- Coupled calculations
  - Fuel evolution
  - Reactor models for fuel cycle simulations
  - Thermal-hydraulics coupling
  - Uncertainty propagation
- Towards a common numerical framework to gather all models

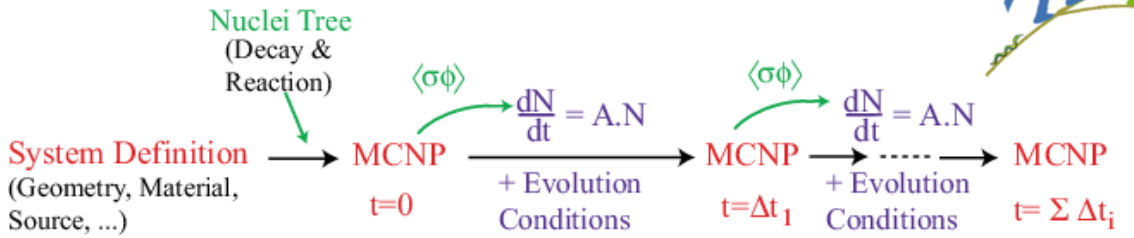
Coupled calculation : fuel evolution

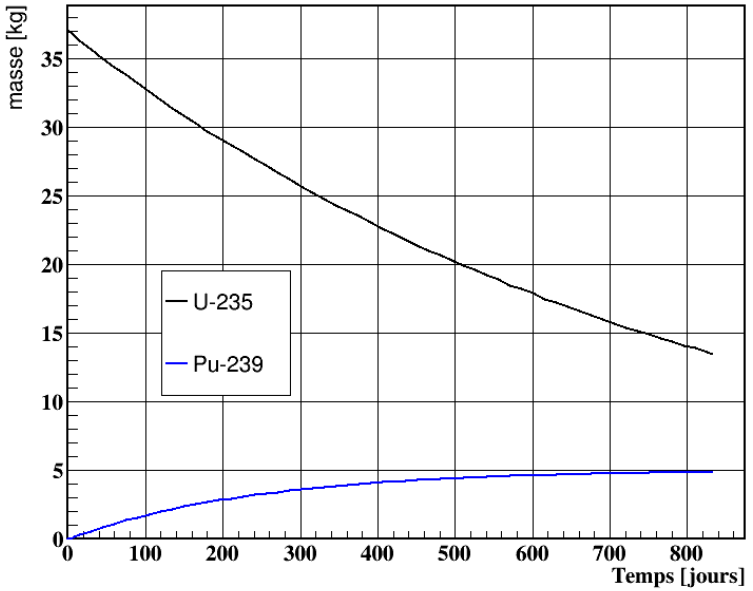
- Reaction rates are necessary to compute the fuel evolution described by Bateman's equation

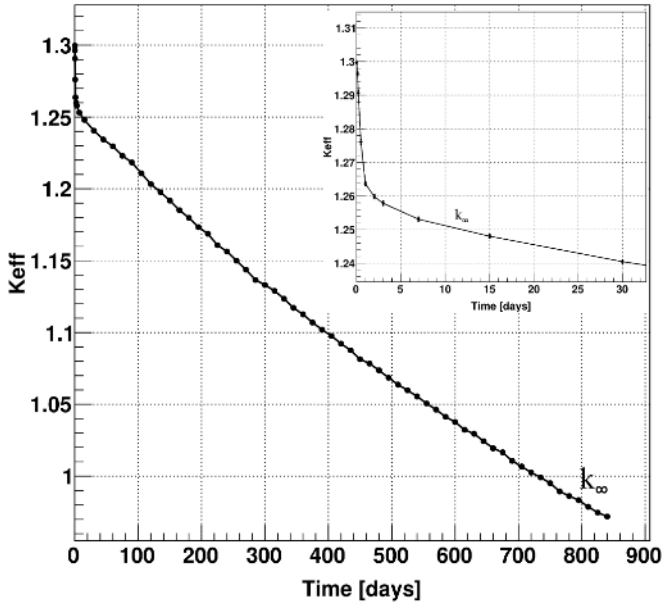
$$\begin{cases} \dfrac{dN_i}{dt} = -\left(\lambda_i + \overline{\sigma_{i,tot}\cdot\varphi}\right)N_i + \sum_{j\neq i}\left(\lambda_{j\to i} + \overline{\sigma_{j\to i}\cdot\varphi}\right)N_j \\ \vec{N}(t=0) = \vec{N_0} \end{cases}$$

Disappearance *Production*

→ The neutron spectrum *(and the reaction rates)* are dependent to the fuel composition







- For prospective studies, fresh fuel composition is unknown !
- Tens of SMURE calculation are needed to determine resources consumption and waste production

- To speed up calculation, use of ANN for :

$$k_{eff}(t) = \boldsymbol{f}\left(\overrightarrow{Pu}, \%_{Pu}, t\right)$$

$$\sigma_i^r(t) = \boldsymbol{g}\left(\vec{N}_0, t\right)$$

Principle of reactor modeling in CLASS (cf. M. Ernoult presentation)

Coupled calculation : fuel evolution

- Reaction rates are necessary to compute the fuel evolution described by Bateman's equation

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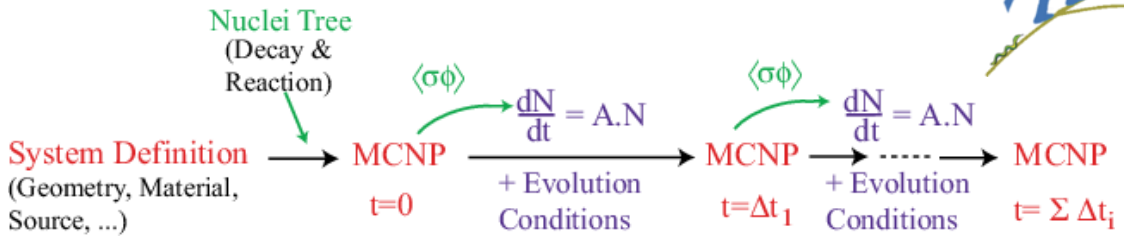
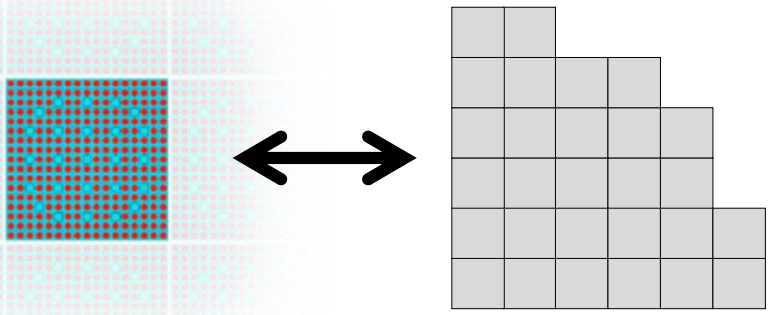
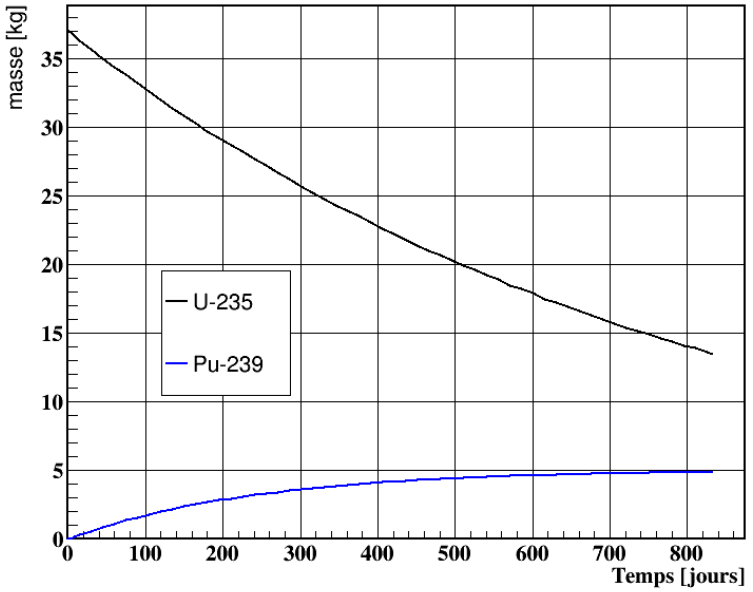
Disappearance *Production*

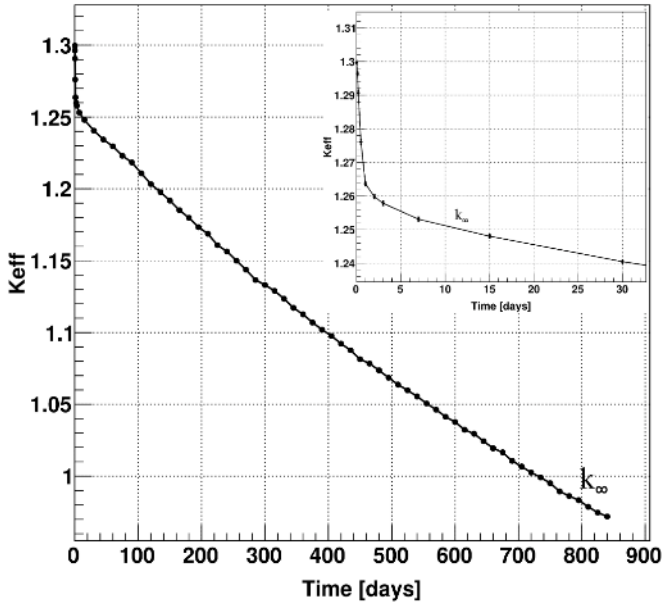
→ The neutron spectrum *(and the reaction rates)* are dependent to the fuel composition

→ Average cross section are also dependent on the localization









→ Assembly calculation are not representative of full core evolutions *Alice Somaini et al. (2017)*

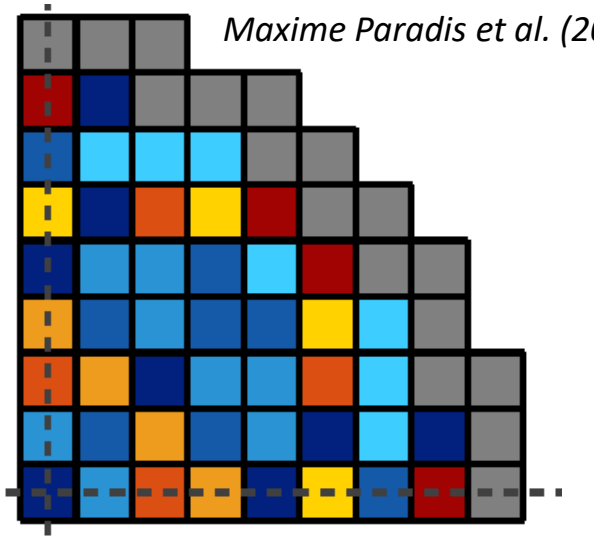
→ Improvement of calculation scheme (collaboration with Polytechnique Montreal)

Fuel evolution : towards full core calculations

- Diffusion calculations mandatory for PWR
  - → Use of academic DRAGON/DONJON tools from Polytechnique Montréal

- New difficulties :
  - Heterogeneous fuel
  - Loading patterns for the core
  - Reactivity follow-up (insure criticality at all time)

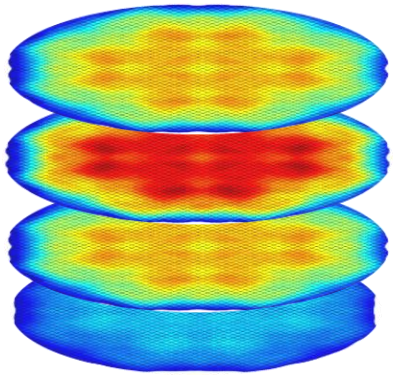
  → A “good” loading pattern insure a “uniform” power distribution at all time – depends on spent fuel properties
  → Goal : identify fresh fuel composition as a function of available material and



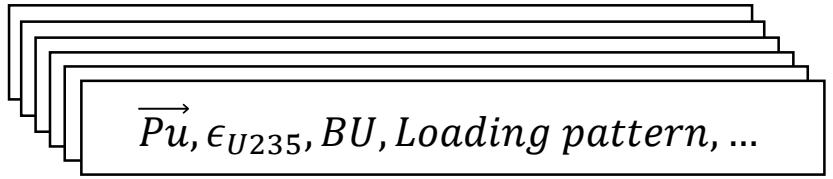
Maxime Paradis et al. (2021)

Example of a UOX/MOX loading pattern

- Use of Machine Learning :
  - → Sampling of possible fresh fuel composition
  - → Power distribution calculation (during evolution)
  - → Artificial neural network for power factor estimation as a function of many parameters

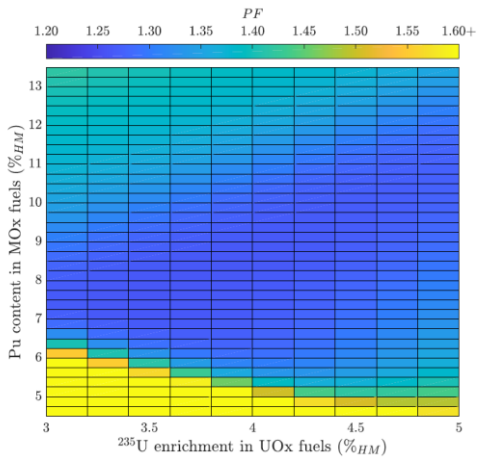


Data base construction
N simulations



$$FP = \frac{P_{max}}{P_{moy}}$$

ANN for power factor



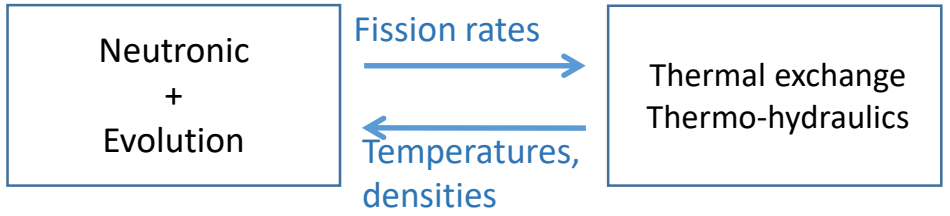
Coupled calculations : transient studies

- Neutron reaction rates are directly dependent on the thermo-hydraulics conditions

$$\Sigma_r \psi = \sum_{isotopes} N_i \int \sigma_i^r(E)\psi(E)dE$$

Isotopic density

Doppler effect on cross sections

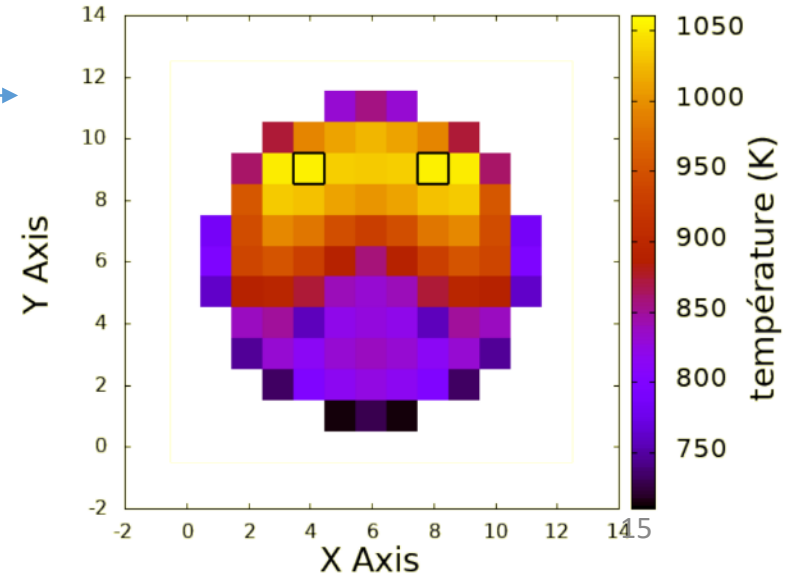


- Any transient study needs a coupling with thermal hydraulics
  - The easiest one : the point kinetics approximation with temperature feedback coefficient → an iterative calculation scheme

$$\Phi(\vec{r},E,t,..) = N(t).\phi(\vec{r},E,\dots) \longrightarrow N(t) \sim N_0 e^{\left(1-\frac{1}{k}\right)\frac{t}{l^*}} \longrightarrow P(t,\vec{r}) \sim N(t).\phi(\vec{r}) \longrightarrow T(t)$$

$$\frac{dk}{dT}$$

- Reactor models based on point kinetics are very limited
  - Specially in accelerated driven system (cf. J.L. Lecouey presentation)
  - Local perturbation (example : control road ejection)



→ Nodal Drift Methods
  - Based on the two group diffusion with delayed neutrons

$$\begin{cases} \frac{1}{v_1}\frac{d\phi_1}{dt} = D_1\Delta\phi_1 - \Sigma_a^1\phi_1 - \Sigma_{1\to2}\phi_1 + (1-\beta)\nu\Sigma_f^2\phi_2 + \lambda p \\ \frac{1}{v_2}\frac{d\phi_2}{dt} = D_2\Delta\phi_2 - \Sigma_a^2\phi_2 + \Sigma_{1\to2}\phi_1 \end{cases}$$

$$\frac{dp}{dt} = \beta\nu\Sigma_f^2\phi_2 - \lambda p$$

Relies on diffusion data

Transient calculations : towards a complete tool box for SMR designs

Assembly calculation *(SMURE)* :
- → *Fuel compostion*
- → *Burnable poison*

↔

Full core evolution :
- → *Reactivity management*
- → *Power factor*

↔

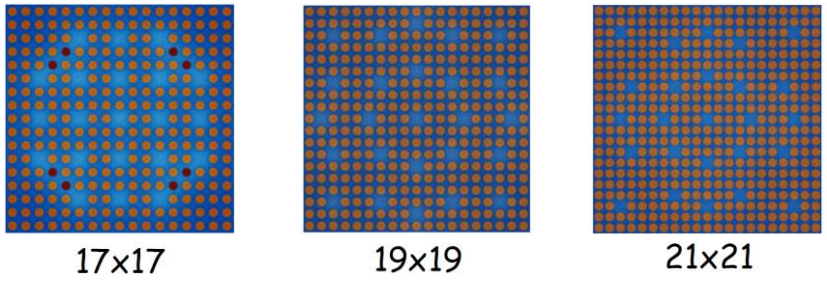
Safety evaluation (NDM) :
- → *Maximal energy released*
- → *Coolant boiling*

➢ Exemple : SMR in thorium cycle cooled with heavy water
- → *Under-moderation necessary for high conversion ratio*
- → *Reactivity monitoring by spectrum modification*

Dilution with light water

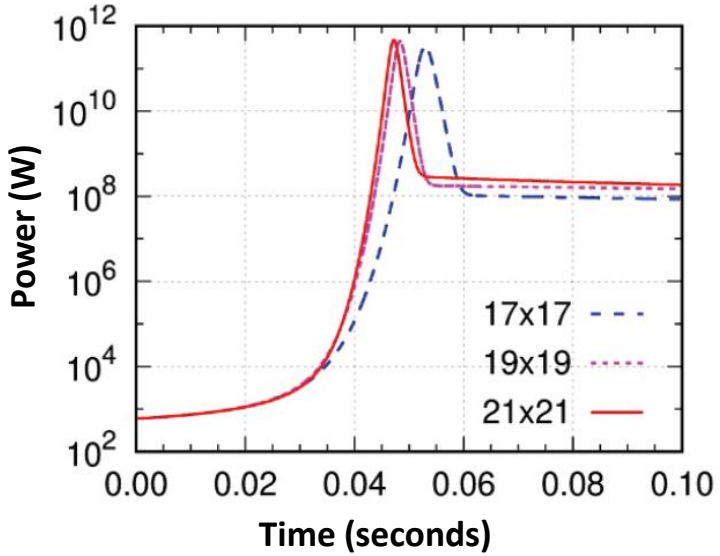
→ Transient study based on Nodal Drift Method

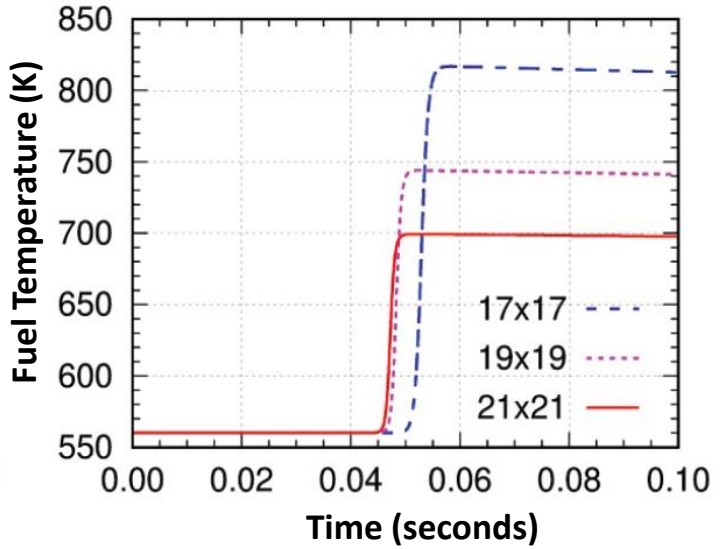
Possible stronger multiphysics coupling (cf. P. Rubiolo)



→ Road ejection

Pierre Prévot et al. (2018)





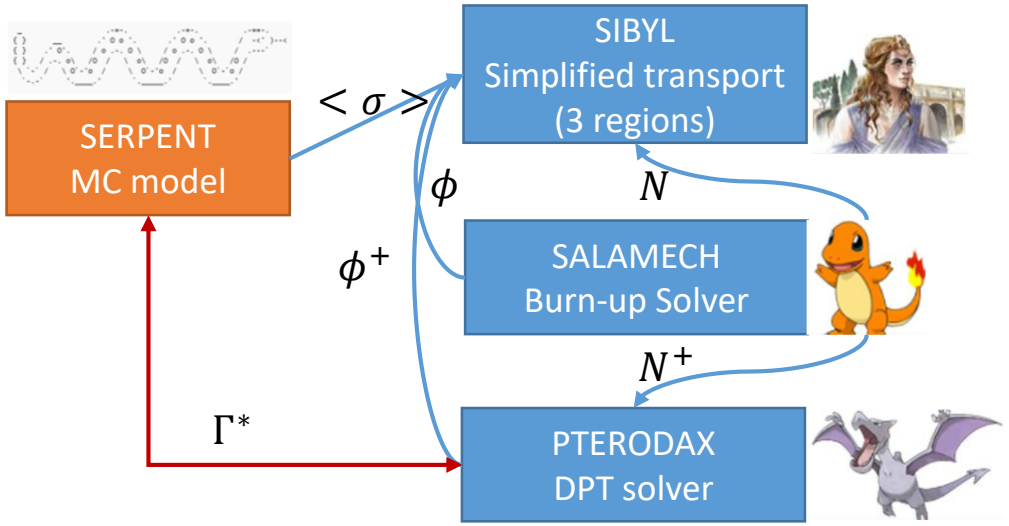
➢ **The goal is not to perform safety studies, but to offer numerical to explore system potentialities**

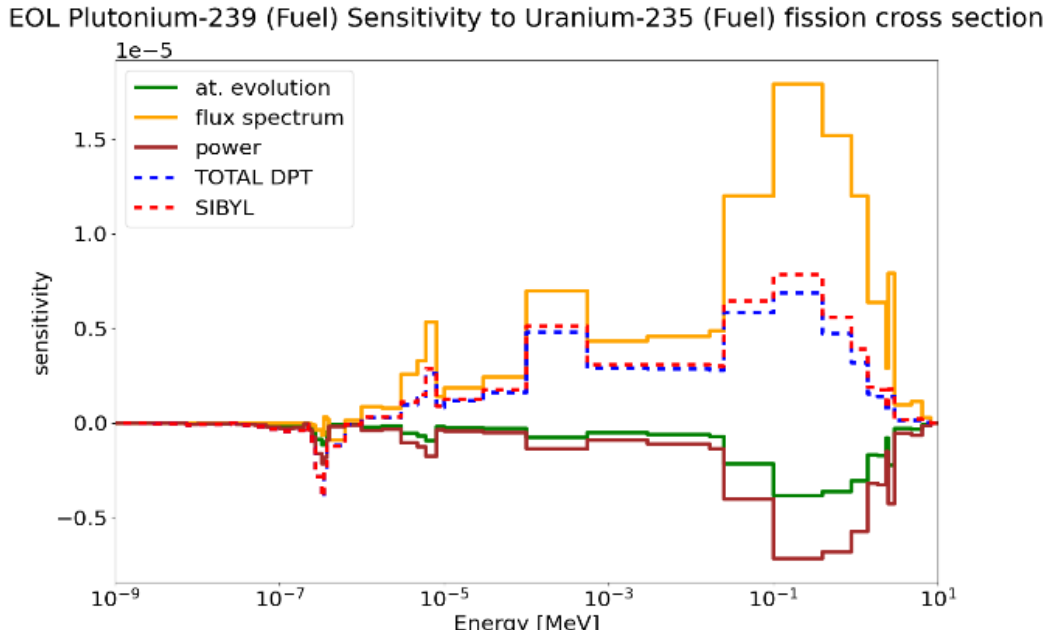
Nuclear data uncertainties for coupled calculations

- Same methodes as for static calculations (GPT and TMC)
  - → *Coupling between Bateman and Boltzomann add difficulties to GPT formalism*

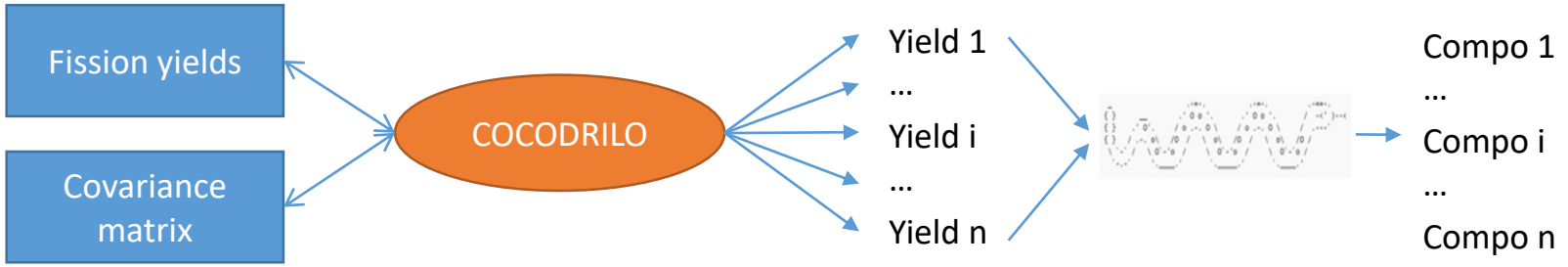
Davide Portinari et al. (2022)

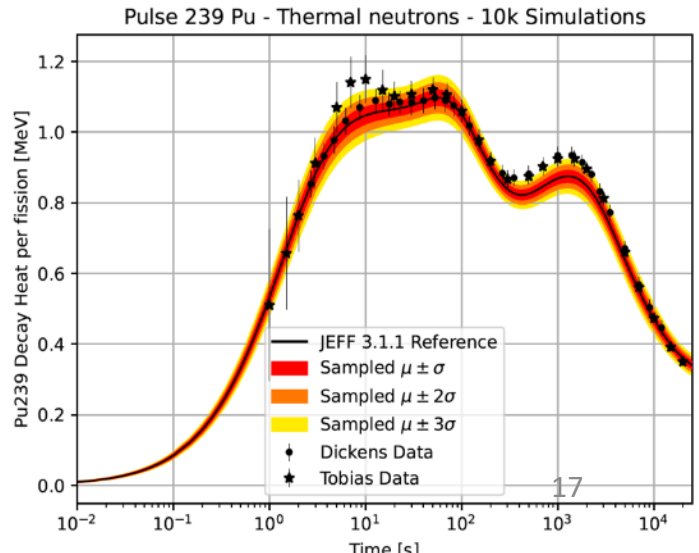
$$S_\alpha = \sum_i \left(\int_{t_i}^{t_{i+1}} N_i^* \frac{\partial (M_i N_i)}{\partial \alpha} dt - < \Gamma_i^* | \frac{\partial B_i}{\partial \alpha} \psi_i > - < P_i^* | \frac{\partial (\sigma_i N_i)}{\partial \alpha} \psi_i > \right)$$





- → *TMC applied to depletion calculation*
- → *COCODRILO development for fission yields and decay heat calculations*





Outline :

- Some take home messages :
  - → Fuel assembly depletion calculation are biased compared to full core depletion calculation
    - Bias ~OK for prospective studies, not OK for precise evolution studies
  - → Point kinetics not precise enough for accidental transient studies
    - Needs of spatial description of the neutron flux dynamics
  - → Uncertainty propagation to depletion calculations needs simplified transport model
    - ***Relies on homogeneous data***
- Boltzmann's equation
- Coupled calculations
- Towards a common numerical framework to gather all models
  - Interest and challenges
  - Some key points
  - As a first step : the OSCAR project

Some huge progress in the 2010s : challenging for knowledge maintenance

- Conclusion of last IN2P3 scientific council : 3 axes to developed
  - → In 2013 :
    - No fuel cycle dynamic simulators
    - Almost no transient studies
    - Beginning of GPT theory (not in evolution)
  - → In 2022 : lot's of innovative methods available to address those issues
    - Sharing a same philosophy
    - Numerous software developed under different standard

- **Complementary work to all current studies on different systems that have to be pursued**

- Specialization with skills developments
  - → **Challenge of sharing, maintaining and archiving our know-how**
    - → Numerical tools are a good option to integrate skills and knowledge

- SMURE and CLASS anchor IN2P3 as a research actor on nuclear energy (at international level)
  - Promotion of our know-how to industrial partners

- **Proposal : pooling numerical developments among a common framework**
  - → Building a "model library" that can be chained for any reactor physic studies
  - → Quantify each model by criteria : complexity/numerical costs/ precision
    Code to code comparison and experimental validation

A common framework to gather our scientific production and knowledge

- Most of reactor physic studies need homogeneous data (multi-level calculation scheme)
  - → Diffusion (for static and depletion calculation)
  - → Nodal Drift method
  - → Modal decomposition
  - → Uncertainty analysis

- Most of reactor physic studies need different solvers
  - → Transient studies = transport + thermal-hydraulics
  - → Evolution = Diffusion + depletion
  - → …

- Different model performances should be compared and validate
  - → MC full core calculations vs transport/diffusion approximation
  - → Modal decomposition vs Nodal Drift Method
  - → TMC vs GPT

- Step 1 : offer interface with transport codes to produce those macroscopic data

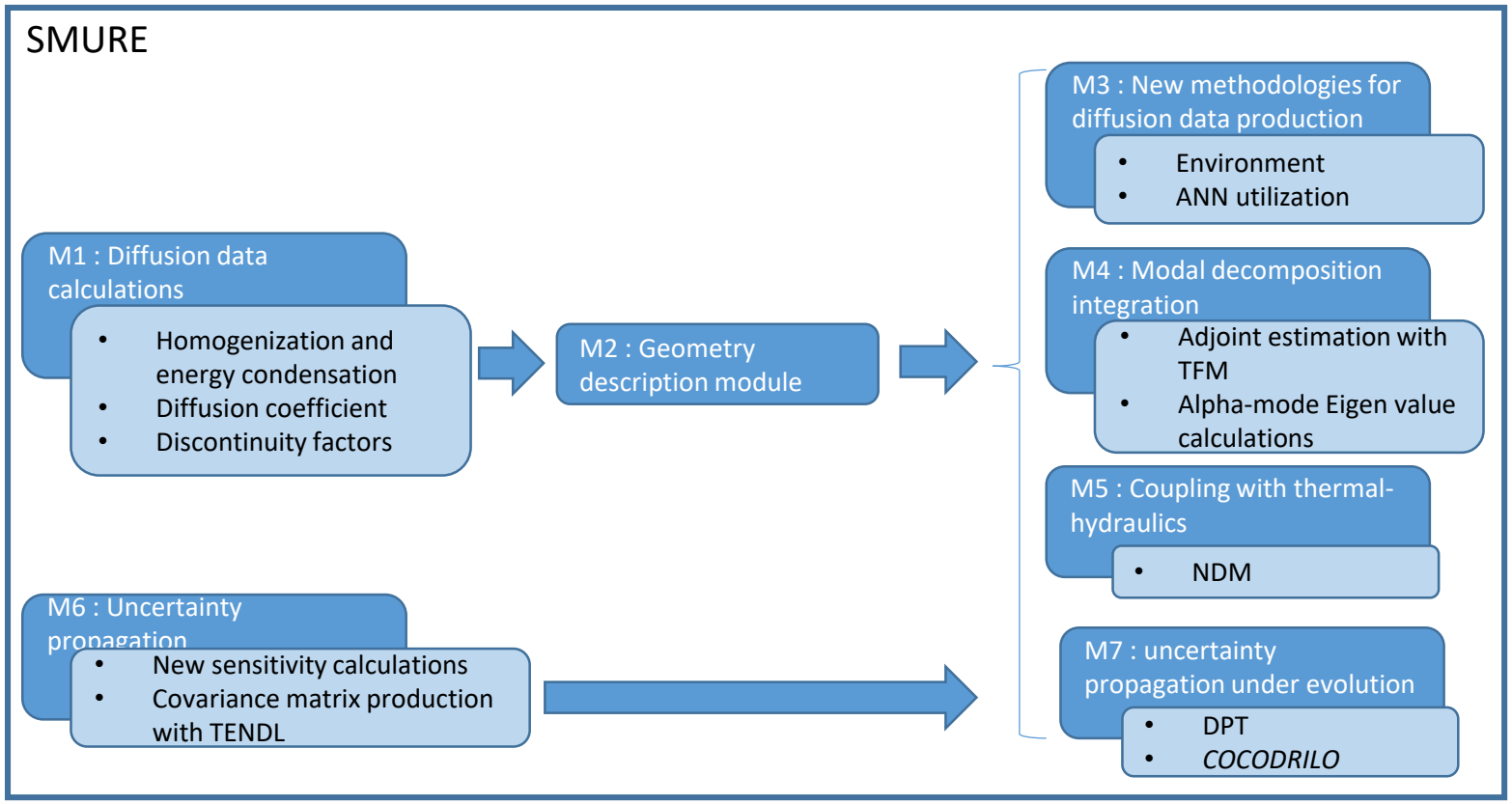
- Step 2 : define a common "form" for chaining all the models together
  - *Necessity of a universal geometry description*

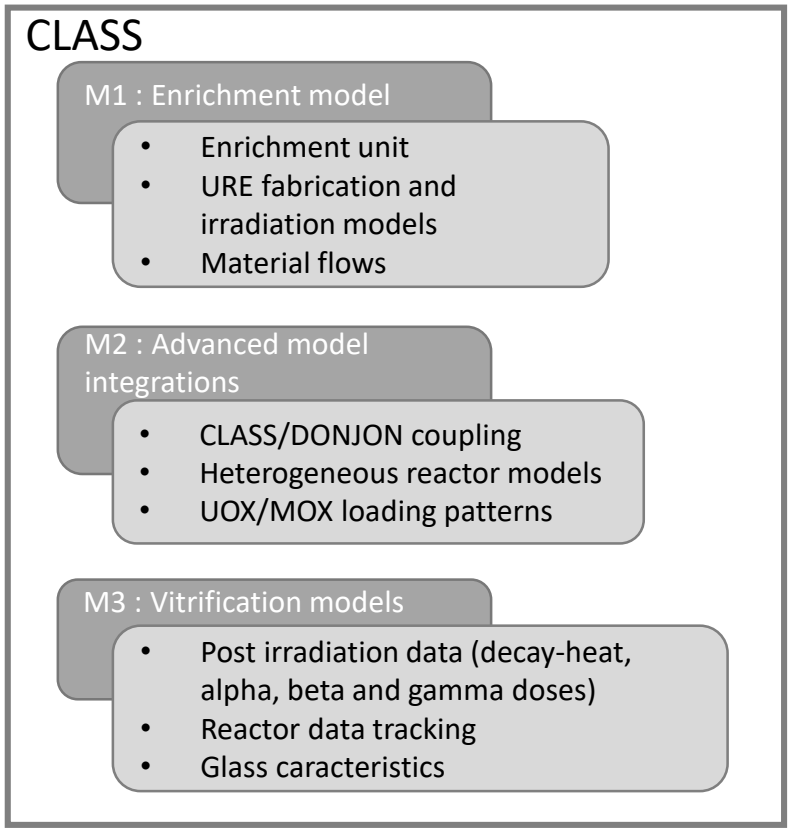
- Step 3 : define a filling system to share our calculations and studies

The goal is not to reproduce existent software or capabilities (like DONJON or SERPENT), but to offer a "tool box" for any kind of studies related to reactor or fuel cycle physics !

To begin with : OSCAR project

- 2022 – 2026 : OSCAR (Outils de Simulations pour les Cycles Avancés et les Réacteurs)
  - → Dedicated to the integration of all recent developments in SMURE and CLASS
  - → Steps and milestones defined in accordance to our human resources





- Those developments are performed for other scientific project (ASSURANCE, SUDEC, OKLO, SIRIUS,…)

  Few project are only dedicated to methods and numerical developpments

From OSCAR project to the future

- 2022 – 2026 : OSCAR (Outils de Simulations pour les Cycles Avancés et les Réacteurs)
  - → Dedicated to the integration of all recent developments in SMURE and CLASS
  - → Steps and milestones defined in accordance to our human resources

- OSCAR project should prepare the future framework
  - → Open access and user friendly (gather external forces)
  - → Easy integration of innovative models
  - → *Integration of external software ?*

- After OSCAR : possibilities will depend on the available resources
  - A numerical platform is a very ambitious and strategic project
  - It can't be done at the cost of physics projects

Numerical resources	Financial resources	Human resources
Complementarity between local and national infrastructure CC-IN2P3 : a huge asset - Exploratory calculation - TMC - Sensitivity studies - Machine Learning	Complementarity between IN2P3 and external funding (30/70) NEEDS program : much more than a financial support	Few Permanent staff (7 in the Oscar project) also involved in other project 11 PhD thesis defended since 2013 3 PhD thesis in progress

Conclusion

- Huge progress done recently in reactor modeling
  - → Driven by system studies (fuel evolution, transient analysis and uncertainty calculations)
  - → Development of numerous software disconnected one from each other

- **Proposal : build a common framework to gather all the developments**
  - Open access and user friendly

1. **Strengthen our understanding of neutronics / reactor physics**
   - → Explore and qualify the unitary "bricks" of reactor modeling
     Neutronic, thermodynamic, and coupled models,...
     - Thanks to experimental validation
     - Thanks to code to code comparison
   - → Use those models for innovative system studies

2. **Enhance our know-how and rationalize our efforts**
   - → Common numerical framework
   - → Promote IN2P3 as a research actor in nuclear energy