Nuclear reactor modeling- Interest of a digital common framework

Abstract :

This paper presents a summary of the research activities carried at IN2P3 on reactor modeling since about 2013. These have mainly been motivated by studies of nuclear systems of interest for resource economy, nuclear waste production minimization or enhanced safety. Over the years, and in accordance with the national and international context, we have therefore studied Pressurized Water Reactors (PWR), Fast Neutron Reactors (FNR) or Heavy Water Moderate Reactors (CANDU), loaded with thorium and uranium fuels. These studies have not only led to prospective reflections about the future of nuclear energy, but also allowed us to acquire solid skills in core modeling. The in-depth analysis of errors, resulting from modelling biases or uncertainties in basic data such as nuclear data for example, has enabled us to develop expertise on the importance of different classical assumptions in reactor simulations. The microscopic study of the behavior of neutrons in a critical system offers the possibility to prioritize the different models according to different criteria such as complexity, accuracy and numerical cost depending on the application study case. In the future, we propose to continue our efforts on advanced system modeling (especially on the treatment of interfaces and the production and use of scattering macroscopic data), to offer relevant coupling schemes with thermal-hydraulics and fuel evolution, and to push forward the methods of sensitivity calculations and uncertainty propagation. In order to rationalize our efforts in numerical development and to increase the visibility of IN2P3, we propose to integrate all our numerical developments for reactor physics within a numerical framework whose format is still to be defined. The objective of such a proposal is to offer a library of models of different complexity, all characterized by the confrontation with experiments or by clever code-to-code comparisons.

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Introduction: an academic vision for reactor physics research

The involvement of IN2P3 laboratories in nuclear energy research, and more particularly in the modeling of nuclear power reactors, began around 1995, following the Bataille's law. These beginnings were devoted to carry out numerous studies on several types of systems (fast and thermal spectra in the uranium and thorium cycle) while developing powerful numerical tools for reactor physics. Since the mid-2000s, the development of SMURE [Mep] (SERPENT/MCNP Utility for Reactor Evolution) has allowed us to integrate most of the knowledge and skills developed in this field at IN2P3. In addition to scientific production (see the selection of published paper in the bibliography section), this research has helped to improve the content of the training programs offered by the IN2P3 laboratory teams and to contribute to the societal debate on the future of nuclear energy.

Recent events and media publications show that the deployment or not of new reactors and the conditions for the development of nuclear energy are still under discussion in the decision-making spheres. In a decade, the international context for the development of nuclear energy has been completely modified at least twice. Before the Fukushima accident, projections for 2050 were very ambitious and showed a strong risk of natural uranium shortage, logically justifying the use of fissile regeneration (plutonium production) and consequently the development of fast neutron systems (Sodium cooled Fast Reactors). In 2018, the re-evaluation of the quantities of natural uranium available and the projections of the starting time of new reactors led, in France, to give up the ASTRID reactor project, pushing back the deployment of RNR to 2090 at the earliest [Chab, 2020]. Finally, very recently, we have witnessed a revival of the nuclear interest in the media, driven by a governmental will to build new reactors - Evolutionary Pressurized Reactor 2 (EPR2), or Small Modular Reactor (SMR) - and to relaunch research on more innovative systems that can implement the transmutation of minor actinides.

In accordance with this evolution, the research projects dedicated to nuclear systems at IN2P3 have put aside fast neutron reactors and the thorium cycle to focus more specifically on shorter-term R&D problems (up to 2050), notably on pressurized water reactors. However, the plurality of technologies studied in the past (PWR [Ern, 2015], RNR [Till, 2019], CANDU [Nut, 2012] [Nut, 2014] but also RSF and ADS [Thio, 2015]) has allowed us to develop a global vision of reactor physics, in particular for coupled criticality simulations with fuel evolution or with thermal-hydraulics. Due to our increased in competence since 2000, our research projects are also evolving towards a more fundamental approach of neutronics. By focusing on the study of physical phenomena of importance according to the studied systems, we seek to quantify the performance of the models used in reactor physics to propose numerical methodologies adapted to the various questions addressed in our research projects.

a. Societal issues related to the future nuclear energy according to different timeframes

There is a certain amount of vagueness among decision-makers about the different possibilities that nuclear energy could offer by the end of the century, which reflects a certain confusion about the availability of materials and the readiness of different reactor technologies.

In the relatively short term (i.e. before 2050 which is the time frame of the energy transition), the only reactors that can be deployed industrially are thermal neutron reactors like EPRs, potentially SMRs. These reactors are fueled by natural uranium that is enriched in uranium 235 in the form of uranium oxide (UOX). They produce nuclear waste (fission products and minor actinides - Np, Am, Cm...) and plutonium that is recycled in France in the form of MOX fuel. Spent MOX fuels are not

currently reprocessed, but since plutonium is today a recoverable material, they are not considered as wastes.

The improvement of safety criteria for reactors in operation requires a continuous improvement simulations' accuracy and thus of modeling performance. We are currently observing difficulties in the modeling of power reactors, especially for the treatment of interfaces, and significant research efforts are devoted to this issue. Moreover, in the context of the energy transition, nuclear reactors are called upon to perform more and more load following. The accuracy of calculations during power transients must therefore be improved, and uncertainties quantified to potentially improve complementarities between nuclear energy and intermittent energies.

The studies of plutonium recycling in various current systems (PWR) concentrate a large part of the research efforts at the national level. The contribution of IN2P3 is presented by the intervention of Marc Ernoult entitled "les scénarios nucléaires en REP et RNR et la gestion du plutonium". All these studies are based on reactor modeling, whether for the simulation of fuel evolution (and to identify the material balances of the reactors) or for the analysis of reactor performance during power transients (in the context of load following or in accidental situations).

In a more distant future (probably after 2070), the deployment of fast neutron reactors (SFR), accelerator-assisted reactors (ADS), or other technologies (Molten Salt Reactors - MSR, for example) has to be considered. These reactors make possible to imagine another use for materials in the cycle, notably through the regeneration of plutonium and transmutation. Because of the difference in the neutrons energy spectrum in these systems (and therefore in their mean free path), the core physics is different from current PWR, requiring the adaptation of methodologies and numerical tools.

Finally, whatever the time horizon, we observe a need of efficient numerical tools for the simulation of reactors, whether those are existing or not. In order to build a wide expertise for all nuclear systems, the philosophy of IN2P3 is to focus on the fundamental physical processes and their prioritization for the physical properties estimation of different systems. Thus, we are able to propose models whose refinement and complexity are adapted to the level of precision of the research problems. The longer term objective is to have a library of models, from the most refined to the most coarse, which would allow us to carry out most of the system studies while identifying the applications where the modeling still needs to be improved.

b. Solving the neutron transport equation as an elementary step to all reactor physics questions

All the problems mentioned above require the ability to calculate all the neutron reaction rates as a function of time and space for a reactor in operation. Indeed, these allow us to estimate the heat depositions as well as the evolution of materials under irradiation, which are elementary quantities for all our studies. To do this, it is necessary to know the distribution of neutrons as a function of energy and position during irradiation. This distribution is described by the neutron transport equation (or Boltzmann equation) which results simply from a neutron balance expressed in Équation 1 where ϕ represents the angular neutron flux (the unknown), $\vec{\Omega}$ the direction variable, $\vec{\mathrm{r}}$ the position, E, the energy, t the time, Σ_{total} (resp. Σ_{s} et Σ_{fiss}) the total macroscopic cross section (resp. scattering and fission), dependent on neutron position and energy, ν the average number of neutrons emitted by fission and dependent on the incident neutron energy, χ the energy distribution of neutrons emitted by fission, $p\left(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}\right)$, the probability that an elastic shock between a nucleus in the medium and a neutron of energy E' and direction $\vec{\Omega}'$ leads to a neutron of energy E and direction $\vec{\Omega}$ and finally S the external sources of neutrons, such as delayed neutrons from decays of some fission products :

$$\frac{1}{v}\frac{d\phi(\vec{r},\vec{\Omega},E,t)}{dt} = -div\left(\phi.\vec{\Omega}\right) - \Sigma_{\text{total}}\phi + \iint_0^{4\pi} d\vec{\Omega}' \int_0^{\infty} dE'\,\Sigma_s(E')\phi\left(E',\vec{\Omega}'\right).p\left(E'\to E,\vec{\Omega}'\to\vec{\Omega}\right) + \frac{1}{4\pi}\chi(E)\iint_0^{4\pi} d\vec{\Omega}' \int_0^{\infty} dE'\,\Sigma_{\text{fiss}}(E')\phi\left(E',\vec{\Omega}'\right).\nu(E') + S$$

Équation 1

When the system is critical, the neutron population is stable in time and the right-hand side of the equation is then equal to 0. Out of equilibrium (under or over criticality), the production of neutrons by fission does not compensate the disappearance. To return to a stationary problem without external source, we alter the fission operator by multiplying the number of neutrons emitted by fission by a scalar λ. The equation then can be expressed as:

$$\lambda \boldsymbol{F}\phi = \boldsymbol{M}\phi$$

where $\boldsymbol{F}$ is the fission operator and $\boldsymbol{M}$, the migration (and losses) one. This equation is an eigen value equation that admits several solutions ϕ_{λ_i}, eigen vectors associated to the eigen values λ_i. The so-called fundamental neutron flux is therefore the eigenvector associated with the smallest eigenvalue which is the inverse of the multiplication coefficient k_{eff}. In a critical power system, the system is stationary and the observed physical flux is the fundamental flux. During a transient, or in the presence of an external source, the measured neutron flux can be decomposed into a weighted sum of the different harmonics. Section 1.c is dedicated to the possibilities offered by this modal decomposition for reactor studies.

In order to numerically solve Equation 1 (stationary) to identify the neutron flux distribution, two families of codes are under developed: "deterministic codes" which consider a discretization of the phase space and "probabilistic codes" (or Monte Carlo) which simulate the histories of a large number of neutrons in order to estimate the average quantities of interest. Today, neither of these two philosophies is fully satisfactory, especially for high-power thermal neutron reactors such as PWRs. Several research actions are carried out today to improve the accuracy of the calculations (see section 1.b) while controlling the associated numerical cost.

The difficulty is reinforced for coupled calculations, whether for the simulation of the fuel evolution or for the simulation of power transients via a neutronic/thermo-hydraulic coupling. The evolution of the compositions during irradiation is given by the system of Bateman equations recalled in Equation 2 where the index i represents a given nucleus, N_i, its atomic concentration (number of nuclides by unit of volume), λ its decay constant and $< \sigma\phi >$ the energy integral of the product of the microscopic cross section and the flux at the location.

$$\begin{cases} \dfrac{dN_i}{dt} = -(\lambda_i + < \sigma_i.\phi >)N_i + \displaystyle\sum_{j\neq i}\left(\lambda_{j\to i} + < \sigma_{j\to i}.\phi >\right)N_j \\ \vec{N}(t=0) = \overrightarrow{N_0} \end{cases}$$

Équation 2

Thus, modeling the evolution of the fuel to calculate the compositions at the reactor discharge (a necessary step to estimate the production of nuclear waste for example) requires knowledge of the spatial and energy distribution in the core. Section 2.b of this document illustrates the difficulties and proposes ways of improvement that are currently under development.

In the same way, for power transient calculations coupling neutronics to thermal-hydraulics (necessary for all safety analyses), the heat deposit distribution is essentially dictated by the fission

rate distribution. Any change in temperature implies an evolution of densities and microscopic cross sections which in return induce a modification of the neutron flux and thus of the heat deposit (see 2.c). An accurate transient simulation then requires the resolution of the Boltzmann equation as accurately as possible.

Finally, the solution of the Boltzmann equation is a crucial step in any reactor physics study. Depending on the scope of the questions addressed, a compromise between the cost of the simulation and the accuracy of the calculations can be found. It is then relevant to distinguish several levels of complexity in the numerical models used at IN2P3 which reflect the diversity and the complementarity of our research. On the one hand, the control of uncertainties and biases in calculations imposes a relatively theoretical and fundamental approach. This reflection on the limits of numerical methods associated with the uncertainties of physical data allows us to feed the industrial R&D to improve or quantify the performances of classical calculation schemes where they are still in default in 2022. On the other hand, the study of future systems does not always require extremely precise computational means, simply because the technological concepts are not yet fully defined. A simplified approach often allows us to propose robust conclusions on the potential of certain technologies to save resources, minimize waste or improve safety, for example. This complementarity allows IN2P3 to approach the subject from both a microscopic point of view, through an ever deeper understanding of physical processes, and from a more macroscopic point of view, through the quantification of properties of systems of interest for the future of nuclear energy.

This document is built around 3 distinct sections. The first two parts focus on current research projects, based on physical modelling issues. The first part deals with "uncoupled" calculations (i.e. without any system feedback induced by a modification of the material properties following fissions). These are the problems of modeling power reactors (specifically the treatment of interfaces), calculations of uncertainties and sensitivities and modeling for kinetics. Then, the couplings with fuel evolution and thermal-hydraulics are discussed.

The third section of this document presents a proposal to gather all the models and numerical tools developed at IN2P3 in reactor physics around a numerical platform that have to be defined and built. The next 10 years could allow a research program dedicated on the one hand to the improvement of the models developed and at the forefront of reactor physics (including experimental validation), and on the other hand to the rationalization of numerical development efforts by integrating all the models within a common numerical framework. The validity and relevance of the models could then be tested through model-to-model comparisons and supported by past and future experimental reactor physics programs carried out by IN2P3, in particular the set of experiments performed at the GUINEVERE facility. The developed models must be integrated in more complete codes and compared to international standards in order to quantify the contributions of IN2P3's research efforts.

All these numerical tools, formalized by a common numerical platform, will also allow to carry out studies applied to very varied systems such as the design of innovative reactors (not necessarily for electricity production like those dedicated to space propulsion or heat generation for example), the search for optimum in the management of reactivity for SMRs or even for the study of OKLO reactors, or the calculation of errors or biases in the current power reactors The integration of sensitivity and uncertainty calculations for each of the models will make possible the "uncertainty by design" approach which will greatly improve the stability and speed of the simulations necessary for the interpretation of experiments and coupled calculations. Finally, the standardization of our tools within the same object will also reinforce the visibility and the expertise of IN2P3 as an actor of the research on nuclear energy.

c. Resources and means

i. Man power

4 laboratories are involved in eactor modeling: these are the LPSC (Grenoble), Subatech (Nantes), LPC (Caen) and IJC-Lab (Orsay). The researchers currently involved in this theme are listed in Table 1.

Tableau 1

LPSC	Subatech	LPC	IJC-Lab
Adrien Bidaud Annick Billebaud Nicolas Capellan Olivier Méplan Alexis Nuttin Pablo Rubiolo	Lydie Giot Nicolas Thiollière	Jean-Luc Lecouey Nathalie Marie François René Lecolley	Xavier Doligez Marc Ernoult

Two points should be noted when looking at this table. First, a large majority of the permanent staff are teacher-researchers (only 3 CNRS staff in Table 1). Second, most of them are also involved in other research projects. Consequently, the degree of involvement of each of them in projects on nuclear systems modeling is diverse. The total involvement represents approximately 4 full time equivalents. We must add the contribution of the PhD students. On average, one to two PhD are defended per year in all the laboratories.

ii. Financial Resources

Since the beginning of our research activities, the financial resources are very diverse: it can be divided in IN2P3 funding (representing between 30 and 50% of our budget depending on the year) to which we must add all the NEEDS projects and industrial research contracts. Thus, since 2013, the projects M2C2, SEC, SUDEC, CINEASTE and MADIFF of the NEEDS program have allowed us to carry out our research projects with our various partners. More recently, research contracts with IRSN, EDF and Technicatome have allowed the funding of PhD training.

Our organization within IN2P3 was built around the Master Project ASSURANCE (2015 - 2019) which was dedicated to the study of SMRs in the thorium and uranium cycle at the reactor and cycle scale. The new Master Project OSCAR, which starts in 2022, provides a framework for the development and valorization of our numerical tools.

1. Solving the Boltzmann equation: current problems and possible improvements

a. Probabilistic and deterministic codes - interest of diffusion

To solve the homogeneous transport equation, the so-called deterministic methods are based on a discretization in the phase space. Although, it is tempting to look for a numerical solution directly on the complete cores of the reactors to be studied (with a characteristic distance of a few meters), a simple consideration on the number of dimensions for meshes necessary for a good representation of the physical phenomena show numerical difficulties that are still too heavy.

The stochastic methods, on the other hand, consist in simulating the histories of a large number of neutrons in the system by drawing randomly the distances traveled, the possibilities of reactions and the products of reactions according to the laws of physics. The behavior of the neutron density as a function of energy and space is then deduced by an averaging over the whole averages

over the set of simulated histories, which are assumed to be independent. However, on large geometries, Monte-Carlo methods are defeated due to the so-called "source convergence" problem which tends to cluster fission sites into "clusters" in the simulation [Dum, 2014]. While it can be physically explained in some special cases [Dum, 2021], this phenomenon greatly complicates the use of Monte Carlo codes for the simulation of high-power (and thus large) thermal neutron cores. For fast neutron systems, cores are sufficiently compact, and the couplings between the different assemblies are strong enough, that simulations of complete cores are possible with Monte Carlo codes.

b. Equivalence transport/diffusion

i. A multi-scale approach for high power thermal reactors

Finally, on an industrial size core such as a typical PWR, both probabilistic and deterministic methods fail. A two-step approach is then classically used. The first one is dedicated to the accurate resolution of the transport equation on small geometries, called "cells", typically representative of a fuel pin or an assembly. This calculation allows the estimation of average quantities on the energy and spatial domain, called macroscopic quantities (or diffusion data). These are introduced in the second step at the scale of the complete core and which considers a simplified equation of the transport: the diffusion equation.

The diffusion equation is obtained by relating the neutron currents to the flux gradient (by the Fick relation $\vec{J} = -D\ \overrightarrow{grad}(\phi)$ where D represents the neutron diffusion coefficient). Thus, the two angular variables have disappeared and the energy and spatial domains are then roughly described (typically, two energy groups and spatial meshes of the size of an assembly fraction). At each instant, the diffusion quantities (macroscopic coefficients and cross sections) depend on the position via a number of intermediate variables (local burn-up and thus composition, temperature, neutron absorbers concentration...). The objective of the cell calculation step is to determine these diffusion macroscopic data as a function of all these variables. Thus, for reactor simulations, a large number of cell calculations are performed in transport to identify the macroscopic cross sections as a function of all the variables of interest for the core. In the second step, the neutron flux distribution, the reaction rates and in particular the heat deposition as a function of the position in the reactor are computed by diffusion calculations with appropriate boundary conditions.

These boundary conditions, which define the flux at the core interfaces, depend on the composition of the materials surrounding the core (reflector) and their neutron properties. The macroscopic cross sections at two energy groups (fast and thermal) of the reflectors depend on the energy of the neutrons coming from the core. Thus, unlike the core meshes whose neutronic properties depend on itself, the neutronic properties of the reflector meshes depend essentially on the adjacent meshes in the core.

ii. Interface modeling difficulties

The interfaces concentrate all the modelling difficulties in systems where the diffusion approximation is necessary, meaning for all the thermal neutron power reactors (i.e. almost all the world's reactors). Indeed, on the one hand, the two-level scheme considers that all the fuel meshes are identical and do not depend on the neighboring meshes (in particular the reflectors for the interface meshes), but on the other hand, the reflector meshes do not depend on the fuel composition, which can however vary greatly, especially in the case of heterogeneous UOX/MOX reactors.

However, since the fuel at the interface is over-moderated, due to the presence of water in the direct vicinity, the macroscopic cross sections considered in the scattering calculation are largely

biased and underestimated. In fact, this local over-moderation leads to a very strong increase of the flux at the interface, leading to a local power peak which can be problematic in some cases.

This local phenomenon is very poorly simulated with conventional two-group calculation schemes due to the method of generating the diffusion macroscopic data. Indeed, by construction, the two-group cross sections are constant as a function of space, without taking into account the over-thermalization at the interface. In the case of MOX reactors, this elevation of flux at the interface is more important than in the case of UOX because of the faster neutron spectrum in MOX fuels (and thus a stronger impact of local over-moderation). It should also be noted that the fissile height of MOX assemblies is slightly shorter than that of UOX due to the presence of a tank to contain the gaseous fission products and the release of helium, which production is more important for MOX fuels. This problem of modeling at the interfaces is the subject of Adrien Rispo's PhD thesis co-supervised with Framatome (CIFFRE thesis).

Similar difficulties can be observed at radial interfaces. The difficulty to produce diffusion values for reflectors, reinforced by the impact of neutron transfer from one mesh to another, leads to (big) difficulties to estimate precisely the radial flux sheet of large power cores (especially when a heavy reflector is present).

Finally, the two-level transport/diffusion scheme, even if it remains the reference today for the study of thermal power neutron cores, is intrinsically limited by the transport step, which produces the macroscopic diffusion cross sections. It could be possible to improve the construction of scattering libraries by taking into account the environment for example.

iii. Interest of a Monte-Carlo/Diffusion coupling, reinforced by the use of neural networks

To improve the description of interfaces, it is tempting to develop specific diffusion libraries for meshes at the interface. The interpolations that allow the calculation of macroscopic cross sections for the core stage could then be different depending on whether the mesh is : in the middle of the core or at the interface. The construction and relevance of this new type of library must then be quantified.

It is possible to go further by considering neighboring meshes in the calculation of diffusion macroscopic data. The description of the neighboring assemblies, in particular the composition of the fuels, may seem delicate to be managed for classical interpolators but neural networks seem to be quite adapted for this kind of exercise. Indeed, unlike the cubic interpolations classically used, the neural network interpolation requires a less dense sampling and thus a limited number of unit cell calculations. The NEEDS MADIFF (Advanced Mathematics for Diffusion) project, which started in 2022, is dedicated to exploring the possibilities of producing diffusion data using innovative methods. It gathers IRSN, Ecole Polytechnique Montréal and IN2P3 on this topic.

c. Reactor kinetics and modal decomposition of the transport equation

Reactor kinetics is the study of the evolution of the neutron flux in transient without any counter-reactions (and generally on the order of minutes). This condition is obtained as long as the modifications of the reaction rates remain sufficiently small not to modify the physical properties of the material (temperature, pressure or composition of materials for example). The understanding of the kinetics of the reactors is not only a necessary prerequisite for all calculations coupled with thermal-hydraulics (presented in part 2.c) but also allows the quantification of certain properties of the systems (such as the measurement of the generation time or of the fraction of delayed neutrons for example). In the presence of an external neutron source, the observation of the temporal evolution of the flux following a perturbation allows to measure the subcriticality levels.

i. Point kinetics theory and its limitations

The point kinetic approximation consists mathematically of factoring the flux as a function of space and time into a product of two independent functions according to Equation 3, with F the spatial component and N the time dependant one

$$\phi(\vec{r}, E, t) = F(\vec{r}, E)N(t)$$

Équation 3

This assumption is quite strong since it assumes that all neutrons are equivalent whatever the site of emission (location of fission) and that a local disturbance at a point of the reactor is instantaneously reflected in the whole reactor. In this approximation, the spatial and energy distribution of the flux, $F(\vec{r}, E)$ (fundamental solution of Equation 1 homogeneous), is not affected by the variation of the global power of the reactor (followed by the evolution of $N(t)$).

As soon as the reactivity is perturbed by a local modification in the reactor, in particular due to a rod movement, the point kinetics approximations are no longer valid and the evolution of the neutron currents during the transients must be considered in order to properly represent the evolution of the flux sheet. This difficulty can be circumvented via a nodal diffusion approach presented in section 2.c.i.

However, even when the geometry of the reactor is not modified, the point kinetics can be faulty, in particular in subcritical systems as it was seen experimentally during the reactivity measurements at the GUINEVERE installation (see the document "La neutronique expérimentale par les méthodes innovantes" and the presentation of Jean-Luc Lecouey). The principle of the different experimental campaigns was based on the temporal monitoring of the count rates of fission chambers placed in several locations in the core for different levels of subcriticality. In these systems, the external source of neutrons implies the presence of harmonics of the flux which add to the fundamental mode (solution of Equation 1). The larger the source (especially in cases where the system is strongly subcritical), the larger the contributions of the harmonics. During a source interruption, the different modes will attenuate with different kinetics.

ii. Modal decomposition

It is then possible to refine the separation of variables formalism by considering the following separation:

$$\phi\left(\vec{r}, \vec{\Omega}, E, t\right) = F\left(\vec{r}, \vec{\Omega}, E\right)e^{\alpha t}$$

Integrating this expression into Equation 1, we obtain the following eigenvalue equation:

$$(\boldsymbol{F} - \boldsymbol{M})F\left(\vec{r}, \vec{\Omega}, E\right) = \frac{\alpha}{v}F\left(\vec{r}, \vec{\Omega}, E\right)$$

And the expression of the flow is then obtained according to :

$$\phi\left(\vec{r}, \vec{\Omega}, E, t\right) = \sum_{i=0}^{\infty} T_i(t)\, F_{\alpha_i}\left(\vec{r}, \vec{\Omega}, E\right)$$

where $T_i(t)$ represents the amplitude of each harmonic of the flux F_{α_i}. The calculation of the harmonics represents a numerical difficulty because of the dimension of the matrix that have to be diagonalized $(\boldsymbol{F} - \boldsymbol{M})$, still induced by the number of meshes (necessary step for the search of eigenvalues and eigenvectors) but this formalism allows to greatly improve the interpretations of the

observations of reactor kinetics (as illustrated in the thesis of Thibault Chevret [Chev, 2016], or in [Vit, 2021]).

The potentialities of this methodology applied to power reactors are numerous. First of all, the observation of the different modes and especially the impact of a disturbance in the core on their spatial shapes allows to anticipate the validity and the transposition of some calculations. The impact of the fuel composition for example (UOX or MOX, or the burnup rate) on the modes would allow to understand very fine behaviors in power reactor kinetics. Ideally, it would even be possible to calculate the sensitivity coefficients of the modes to different parameters, such as the position of the control rods, the boron concentration or even the temperature distribution (see 1.d) for example. This is what Davide Portinari is trying to do in his PhD thesis.

On the other hand, the use of this modal decomposition allows to generate the multi-group diffusion constants for systems far from criticality [Zoi, 2014] [Var, 2020], while the classical process, based on condensation and cross-section homogenization operations, implicitly assumes that the system is always critical. Modal decomposition on reflector diffusion data calculations would also provide a good characterization of the evolution of macroscopic cross sections as a function of the reactor state. The calculations of accidental transients, performed in diffusion, could thus be improved with macroscopic data generated from a modal decomposition.

Today, we have only limited expertise in these methods, which have only been applied to the analysis of experiments at GUINEVERE. To explore the possibilities of this modal decomposition, it is first necessary to develop the numerical formalism, which could mobilize part of our efforts in the coming years.

d. Sensitivities and uncertainties

Since about 2010, the calculations of sensitivities to nuclear data and the associated uncertainties have occupied a non-negligible part of our efforts. As for the flux calculations, we first deal here with the problem of criticality calculations (uncoupled static calculations) before addressing the problem of evolving uncertainties in part 2.b.iii.

There are essentially two methods for propagating uncertainties induced by nuclear data: the so-called Total Monte Carlo (TMC) method and the Generalized Perturbation Theory (GPT). The principle of TMC is to sample randomly some of the parameters of the models used for evaluations, which allows to create a large number of neutron data bases, whose dispersion is representative of the uncertainty of the nuclear data. Then, one has to randomly pick from these evaluations (taking into account the correlation matrices when available) to perform a large number of Monte-Carlo neutron transport calculations. This method, very expensive numerically, allows to calculate the errors of the neutron quantities of interest related to the evaluations of the nuclear data (cross sections, fission yields, fraction of delayed neutrons etc...) associated to a nucleus. It is however difficult to understand what are the main sources of uncertainties (which reaction and why) in front of the numerous counter-reactions in reactor physics.

We then studied the possibilities of applying the generalized perturbation theory on thermal and fast neutron reactors in order to understand the possibilities and the limits of such a theory [Par, 2019], [Bid, 2017]. This method, although less accurate, is much faster, especially as soon as one has to study uncertainties on local observables, different from the multiplication coefficient or the mean generation time for example.

These two methods have very different philosophies and the information provided by the two approaches is complementary. While the perturbation theory is based on a sensitivity calculation

(which can be seen as a partial derivative calculation), the TMC method looks for a global uncertainty by taking, by construction, all possible compensations. Thus the first method offers an analytical tool to physicists to understand and prioritize the importance of the different physical processes, while the second one allows to quantify precisely the uncertainty induced by the bad knowledge of the core.

i. Adjoint equation, sensitivity and uncertainties

We can link the variance of an observable (here the neutron multiplicative coefficient k_{eff}) to the covariance matrix of the parameters (here the cross sections σ_i) using the vector of sensitivity coefficients (written here S_σ) as in Equation 4. The sensitivity coefficients are defined as the relative change in the observable induced by a relative change in a parameter.

$$var(k_{eff}) = S_\sigma^t . cov(\sigma_i, \sigma_j) . S_\sigma$$

Équation 4

To calculate the sensitivity coefficients, we often consider the equation added to the Boltzmann equation (where ϕ^+ represents the adjoint flux and $\boldsymbol{F}^+$ and $\boldsymbol{M}^+$ the mathematically adjoint operators of the fission and migration operator):

$$\lambda \boldsymbol{F}^+ \phi^+ = \boldsymbol{M}^+ \phi^+$$

It can be shown that the sensitivity coefficient of k_{eff} to a given cross section can be calculated according to the expression :

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

Thus, the knowledge of the flux and adjoint flux allows us to simply calculate the sensitivity vectors. By knowing the covariance matrix of the cross sections, tabulated in the nuclear data (see Maëlle Kerveno's presentation entitled "Measurement, uncertainties, calculations") it is then possible to quantify the uncertainties given by the nuclear data.

The solution of the adjoint equation is relatively simple with deterministic methods since the adjoint operators are obtained simply by transposing the direct operators. Deterministic codes have thus for a long time had an advantage over Monte-Carlo methods since they were able to calculate the direct and adjoint fluxes in the same way.

ii. Monte-Carlo sensitivity calculations

The revenge of Monte-Carlo codes on sensitivity and uncertainty calculations has taken place very recently (mid-2010s) via the development of innovative methods to calculate sensitivity coefficients by considering the physical interpretation of the adjoint flux, which can be seen as the share of reactivity carried by a neutron in an elementary volume of the phase space [Auf, 2015]. The Iterated Fission Probability method, which is based on the measurement of the number of neutrons descending from an initial neutron after several generations, then allows a direct estimation of the adjoint flux for Monte Carlo calculations of sensitivity coefficients.

The generalized increase in computing power, and in particular in the memory associated with Monte Carlo calculations, makes it possible to temporarily store the links between different generations of neutrons during criticality calculations and thus to calculate sensitivities to observables other than the k_{eff}. A part of the NEEDS SUDEC project (CNRS/IN2P3, CEA and IRSN), led by A. Bidaud, is dedicated to the exploration of these new possibilities offered by the SERPENT2 code. One of the objectives is to calculate the sensitivities of different reaction rates to new parameters which can be

of very different natures. We will particularly note the parameters of nuclear data as close as possible to the evaluation parameters (such as resonance parameters or double differential effective cross sections for example [Auf, 2016]) or, on the contrary, physical parameters other than neutron ones such as temperatures.

One of the main difficulties of this work is to ensure the convergence of the Monte Carlo for the sensitivity calculations. For example, for thermal neutron PWR type power cores, the computational effort to obtain a well-converged solution can be very costly. This is what Pamela Lopez observed during her PhD thesis when calculating the sensitivity to different effective cross sections of the power distribution in a PWR (in particular to the inelastic effective cross section of U-238, measured recently by the IPHC). These power distributions are particularly sensitive to diffusion reactions which have much less impact on criticality for example. Adding the neutron dilution effect due to the large size and thus to the relative reduction of the casing volumes, these sensitivity coefficients are particularly delicate to evaluate. The demonstration of the link between the large number of generations to be followed to obtain the sensitivities of the power distributions in Monte Carlo and the high dominance ratio remains an open question to our knowledge.

iii. Modal sensitivities to accelerate the convergence of calculations

Partially to address this issue, we propose to revisit the work started at Berkeley by Manuele Aufiero on the calculation of temperature sensitivities of neutron modes by applying the methodology to nuclear data. This approach seems to have important advantages from a statistical point of view. Indeed, the modes being defined everywhere, the perturbations of the life of each neutron, wherever it is, have a contribution on all the modes studied. Thus, the accumulation of statistics must be much faster for the calculation of the sensitivities of these modes than for the sensitivities of the neutron density in a reduced volume of the geometry (and space in energy...).

On the other hand, the calculations of sensitivity of the different modes to temperature would also accelerate the coupled neutron/thermodynamic calculations. The sensitivity coefficients would allow to optimize the number of resolutions of the neutron transport in order to realize only those which are essential (where the sensitivities are exacerbated).

2. Coupled modelling - Review of nearly 20 years and future prospects

a. SMURE

i. Brief history

The development of SMURE started around 2003 in order to interface firstly the Monte Carlo transport code MCNP and then the SERPENT code with its own evolution module in order to solve the evolution equations mentioned in the introduction (Equation 2). The first system studies at IN2P3 were aimed at exploring the reduction of waste production with systems such as PWR, CANDU or RNR-Na in thorium cycle. These studies were carried out in particular during the PhD theses of Franco-Michel Sendis, Perrine Guillemin and Julie Brizi, and naturally evolved towards the question of americium and plutonium recycling, especially in the PhD theses of Robert Sogbadji and Marc Ernoult.

The development of couplings with thermo-hydraulics was quickly considered, within the PhD thesis of Nicolas Capellan, in order to build tools and methodologies of interest for the estimation of safety performances.

Although these studies provided very enlightening results on the different advantages and drawbacks of the different possible systems, they showed methodological limitations which were identified and overcome in more fundamental work. Thus, for the simulation of power reactors in the

context of anti-neutrino studies (Anthony Onillon's PhD thesis), particular attention was paid to the calculation scheme used in order to control the modeling uncertainties. This reflection on the representativeness of assembly calculations with respect to irradiations in the core was continued in the thesis of Alice Somaini. Finally, the academic tools development for the design and safety of innovative reactors have been completely taken up in the PhD thesis of Pierre Prévot and applied to SMRs loaded with thorium.

The study of fuels after irradiation and more generally the characterization of alpha, neutron, beta and gamma spectra of all materials was made possible during the PhD thesis of Baptiste Leniau via the integration in SMURE of a module allowing the calculation of all types of post-irradiation data.

All these developments have allowed us to acquire an expertise in the simulation of fuel evolution, which is necessary for any prospective study on the nuclear power of the future. In particular, this has enabled us to develop reactor models in the CLASS code, a cycle physics tool that allows us to study different reactor deployment scenarios, which are presented in Marc Ernoult's contribution to this scientific council.

ii. Advantages, current limitations and projects

In addition to the historical interest, SMURE is a code that allows the coupling between Monte-Carlo codes and an evolution module offering a very high variability of use. The interface with MCNP or SERPENT2 allows, for example, to modify the geometry during the evolution and to realize any kind of evolution under constraints. For example, for SFR calculations, it is possible to simulate the reloading and displacement of fuel assemblies during the evolution in order to take into account the real history of the assemblies positioning. It is also possible to perform boron tracking for PWR assembly evolutions, or even to slave the position of control rods to criticality for SMR studies.

SMURE being based on a resolution of the transport equation by Monte-Carlo methods, it suffers however from the same limitations as the latter. Thus, it is not possible to simulate a complete PWR reactor in evolution without requirement unreasonable calculation costs. The simulations of power transients suffer from the same limitation. In both cases, the use of diffusion remains essential but we do not have a solver that can be easily coupled with SMURE. The production of diffusion data in Monte-Carlo is now possible with the SERPENT2 code, but the proposed algorithms must be used with caution because their validity is not always established. Transient calculations in diffusion are today performed with an internal module named sNDM (Nodal Drift Method) [Nut, 2016] and we plan to push its use to evolution calculations on complete cores and integrate it with SMURE.

b. The evolution of fuel: towards the consideration of the core scale

i. The required models for fuel cycle dynamic simulations

For all prospective studies on the production of waste or the consumption of natural resources, it is necessary to be able to estimate easily and quickly the masses of fuel to be loaded in the reactor according to the isotopy of the available materials. It is equally important to be able to calculate the evolution of these materials during irradiation precisely. Mathematically, it is necessary to estimate the functions $\boldsymbol{f}$ and $\boldsymbol{g}$ which respectively estimate the fissile content to be inserted in the fuel as a function of its isotopy and the burn rate of the reactor and the fuel composition as a function of the initial composition and time such that :

$$\%_{Pu} = \boldsymbol{f}\left(\overrightarrow{Pu_{stocks}}, T_{irr}\right)$$

$$\vec{N}(t) = \boldsymbol{g}\left(\vec{N}_0, \%_{Pu}, T_{irr}\right)$$

where $\%_{Pu}$ represents the fissile content in the fresh fuel, $\overrightarrow{Pu_{stocks}}$, the isotopic composition of the available fissile materials, T_{irr}, the irradiation time, $\vec{N}(t)$ the fuel composition as a function of time ans $\vec{N}_0$, the initial fuel composition.

The use of SMURE allows to estimate very precisely the functions $\boldsymbol{f}$ and $\boldsymbol{g}$, at the cost of a relatively high numerical power. To speed up the studies, the use of machine-learning and in particular neural networks allows us to numerically estimate these functions from a large number of previously performed evolution simulations [Len, 2015]. This approach then allows us to build accurate reactor models for use in the CLASS physics code (see Marc Ernoult's contribution).

The use of neural networks allows us to numerically reproduce the evolution of code such as SMURE very efficiently in terms of accuracy and speed. However, these advanced regression techniques, as accurate as they may be, are based on initial data that are subject to errors. For thermal reactors, the evolutions are performed on infinite assembly geometries, without reactivity control and without taking into account the neighbors (like the cell calculations of two-level schemes). Alice Somaini's thesis showed that the omission of core-scale physics brought large modeling biases to the estimates of inventories at unloading (more than 10% on minor actinide inventories, several % on plutonium and uranium isotopes) [Som, 2016].

ii. Use of the Montreal tools: DRAGON/DONJON

To improve the fidelity of the fuel evolution simulations, it is possible to use two-group diffusion calculations to take into account neutron leakage and thus the position of the fuel in the core in the modeling. Since diffusion calculations are assumed to be inexpensive, we have built models for fuel construction and irradiation that take into account the core scale in a collaborative project with the École Polytechnique de Montréal [Gui, 2021]. The difficulties of implementation are multiple: it is necessary to identify the loading plan, to correctly simulate the monitoring of the reactivity and to identify the end of the irradiation according to the initial compositions, but these have been overcome recently, allowing an accurate and rapid evolution of the fuels.

To identify acceptable loading plans and initial compositions that guarantee an acceptable radial power factor, we have developed a numerical approach based on the use of neural networks [Par, 2021] which requires the construction of a core-scale simulation database.

iii. Uncertainties propagation to depletion calculations

As for the un-coupled calculations, the modeling biases can be considered as errors that must be compared to the uncertainties induced by the nuclear data. For uncertainty propagation to depletion calculations, one must then take into account the coupling of the Boltzmann and Bateman equations in generalized perturbation theory which greatly complicates the formalisms [Sab, 2013] [Bid, 2017]. The TMC method remains advantageous since it is relatively easy to implement and remains very accurate (within stochastic uncertainties) but it requires significant computational resources.

The PhD work of Davide Portinari on the implementation of the Depletion Perturbation Theory (DPT) applied to the high flux reactor of the ILL shows very satisfactory agreements with direct calculations, even if many compensations between terms of opposite signs are present. We note for example that an increase in the fission cross section will result in a decrease of the flux level to keep the power constant, leading consequently to a decrease of the captures on U-238 and thus a lower production of Pu-239 in the end. By combining these group sensitivities with the covariance matrices, it is now possible to calculate the uncertainties and compare them with "Total Monte Carlo" solutions.

In parallel, in order to quantify the impact of uncertainties on post-irradiation data, the COCODRILO code, based on the use of the Total Monte Carlo method, has been under development since mid 2020 at Subatech. It is dedicated to the impact of uncertainties in decay data (fission yields, average energies and decay constants) on the uncertainty of the residual power. COCODRILO is a set of python scripts coupled to the SERPENT code, which currently allows to produce independent fission yield files, which are then used for evolution calculations. An optimization of the scripts has been performed in order to reduce the computation time and the memory space needed at the IN2P3 computing center and developments are in progress for applications to uncertainties of other decay data.

c. Reactor dynamics: a first step towards multi-physics

The study of the potential of reactors for the future of nuclear energy must necessarily address transient behavior, especially in accidental situations. Our objective is not to carry out advanced safety studies on a given system, but on the one hand to explore the possibilities and limits of innovative concepts during typical transient scenarios, and on the other hand to develop methodologies which allow to study these transients properly. Indeed, if scenario studies enlighten us on the interest of different systems in front of resource and waste issues, the study of reactor dynamics enlightens us on the possibilities for industrial deployment and their use in a fleet solicited to perform load following [Pre, 2017].

In the context of power transients, it is necessary to take into account the counter-reactions of the system following a variation of the fission rates in the core. Indeed, these directly impose the heat deposits that set the temperature distributions from the coolant flow conditions. The temperatures and densities of the materials influence the neutronics, due to the modifications of the microscopic cross sections induced by the Doppler effect, as well as the macroscopic cross sections induced by the variations of atomic concentrations as a function of the temperature.

One can distinguish several degrees of coupling between the physical processes of neutronics, thermodynamics and thermohydraulics. Here, we treat only a "weak" coupling where the thermal and neutronic equations are solved sequentially, but it is possible to consider stronger couplings. They are the subject of a specific contribution for this scientific council and are treated by Pablo Rubiolo in his paper entitled "Multi-physics couplings".

i. From point kinetics to nodal kinetics

We have presented earlier in this paper the formalism of point kinetics which assumes that the spatial distribution of neutrons varies in a homothetic way when the system is modified and perturbed. But very often, energetic spatial effects are not negligible and the behavior of fast neutrons must be differentiated from the behavior of thermal neutrons.

To overcome this difficulty, the equations of nodal kinetics are often considered. The principle is to discretize the geometry of the reactor and to consider the time-dependent diffusion equations. We then have, for each mesh of the system, the system of Equation 5 which governs the fast and thermal flows (where n_i and v_i are the neutron density and the averge neutron speed of each group *i* – 1 for fast neutrons, 2 for thermal neutrons) as a function of the diffusion coefficient (D_1 and D_2), of the macroscopic cross-section of absorption for each group (Σ_a^i), of the macroscopic fission cross section (in that case, only for thermal neutrons, Σ_f^2) and finally of the transfer macroscopic cross-section (or slowing down, $\Sigma_{1\to2}$). In this equation, we made appear the precursors of delayed neutrons (here only one group) whose concentration is noted p and its decay constant λ.

$$\begin{cases} \dfrac{dn_1}{dt} = D_1 v_1 \Delta n_1 - \Sigma_a^1 n_1 v_1 - \Sigma_{1\to 2} n_1 v_1 + (1-\beta)\nu\Sigma_f^2 n_2 v_2 + \lambda p \\ \dfrac{dn_2}{dt} = D_2 v_2 - \Sigma_a^2 n_2 v_2 + \Sigma_{1\to 2} n_1 v_1 \end{cases}$$

Équation 5

The equation that governs the population of delayed neutron precursors is the following:

$$\frac{dp}{dt} = \beta\nu\Sigma_f^2 n_2 v_2 - \lambda p$$

ν beeing the number of neutron emitted by fission and β, the delayed neutron fraction.

In these expressions, we find again the difficulty of calculating diffusion macroscopic data with Monte-Carlo codes and especially with SMURE. The use of SERPENT2 on complete geometries allows us to consider transient calculations on SMR. This is notably what was done in Pierre Prévot's thesis for the dimensioning of water-cooled SMRs loaded with thorium [Pre, 2017]. It is also this kind of methodology that can be used for the design of innovative reactors design for other application than electricity production such as the Krusty space propulsion reactor.

ii. Thermal hydraulic coupling

The calculation of the temperature field can be done with several tools, more or less complex. The objective is to adapt the level of complexity to the desired accuracy of the global studies. The calculation of the power distribution evolution during transient being carried out here under the diffusion approximation, it does not seem relevant to have a very fine representation of the thermal-hydraulics to calculate the temperature distribution. Advanced multiphysics schemes allowing to describe the processes at work at the microscopic level and at the nano-second scale and based on CFD calculations for the description of the flows are presented in the contribution of Pablo Rubiolo.

Two numerical tools integrated to SMURE for the calculation of temperatures can be considered. The first one, named BATH (for Basic Approach of Thermal Hydraulics), is a module developed at IN2P3, which solves the heat equations in 2 dimensions (R-Z) considering several approximations to keep a simple formalism (radial conduction transfer in the pellet, incompressible heat transfer model,...). The second one is the COBRA-EN code, a sub-channel code available at the NEA. The differences observed between the two couplings show that for flows respecting the safety criteria, the simplifying assumptions of BATH are justified and allow a good agreement with an industrial sub-channel code. For degraded flows, BATH predictions are less accurate but acceptable. In particular, the failure by excess of the critical heat flux is correctly predicted by BATH.

This coupling has been used for the design of an SMR fuelled with Th/U and Th/Pu fuels. The objective was to identify assembly configurations that would make it possible to satisfy different objectives, such as maximizing plutonium consumption or uranium production, maximizing the burnup rate, while proposing innovative reactivity management in order to limit the number of reloads. The ideal is for an SMR to manage reactivity without boron and without partial reloading. Once the technological solutions have been proposed, the safety performances of the cores have been evaluated using these couplings to simulate typical transients such as a cluster ejection [Pre, 2017].

This approach can be used for the academic design of any other type of innovative SMRs, whether or not they are power plants.

3. Towards a common digital framework

The first two parts of this document have recalled that the study of innovative systems has allowed IN2P3 to develop different models for reactors and to build up an expertise on the potentialities of the different technologies, both in terms of resources savings and waste management, as well as in terms of considerations relevant to safety and operation. The analysis of the performances of these different models, and in particular their accuracies, compared to the uncertainties induced by the physical parameters (specifically the nuclear data) logically led us to study the behavior of neutrons in critical systems via a fundamental approach, as close as possible to the physical phenomena. Comparisons of models performed on well thought benchmarks allow us to quantify the impact on the accuracy of calculations of each approximation and assumption depending on the application case. For example, fuel evolutions considering only the assembly scale have been compared to evolutions taking into account the core physics scale. These comparisons make it possible to distinguish the cases where the "assembly" approximation is acceptable and leads to limited biases (as in the case of UOX, for example), from the cases where the consideration of the core scale is indispensable (as in the case of heterogeneous reactors, for example).

Moreover, the experimental physics program carried by IN2P3, initially built for the measurement of subcriticality in ADS, has allowed us to experimentally highlight the modeling flaws of some very classical approaches (such as point kinetics for example). The set of data produced by the GUINEVERE installation constitutes a fine collection of criticality and kinetic experiments that can be used to test and validate a certain number of numerical methods, specifically in the field of fast and epi-thermal neutrons. The variability of the core configurations studied (see contribution of Jean-Luc Lecouey) represents an important richness of these experimental data. For example, the very fast configurations produced with metallic fuels have shown very strong couplings between the core and the concrete walls of the reactor building, while other configurations with graphite to thermalize the neutron spectrum have shown almost no influence of reflectors. The confrontation of modeling and experimentation offers a unique opportunity to measure the progress in modeling as a function of reactor parameters.

This approach, which consists in studying at the microscopic level the behavior of neutrons in a multiplying medium to control numerical uncertainties, will be continued in the future. System studies, in particular the modeling of EPRs and SMRs, loaded with UOX and MOX fuels, should also continue to mobilize a large part of our research efforts. The degree of finesse and precision of the models implemented must be adapted to the precision desired for each future study.

In order to simplify these future studies, to have the right numerical tools according to the different scientific problems but also to capitalize all our developments, we propose to collect the different models within a common numerical framework. The challenge is to make available the unitary bricks represented by the different solvers of the different equations and to be able to connect them to each other for any reactor physics modeling. The accuracy and the field of use of each of the solvers must be specified as well as the numerical costs necessary to precisely identify the accuracy/simplicity/computational needs of each of them.

It is worth noticing that the models we plan to integrate into this effort are of various natures and at very different stages of development. For example, the couplings allowed by the SMURE environment are for some very advanced and are directly available. On the other hand, the formalisms for diffusion, nodal decomposition or uncertainty and sensitivity studies are still in their infancy and cannot yet be directly integrated into a numerical platform.

The rest of this section details the philosophy, the objectives and the benefits as well as the difficulties of the implementation of such an approach.

a. A library of "models" whose performance is quantified

We have seen in the first part of this document that the solution of the transport equation, for thermal reactors, is done by a two step process, via a transport calculation to produce diffusion data and then a core calculation. If it is possible to perform a simulation with only one step for small cores or fast reactors in criticality calculations, it is very often not possible for coupled calculations. Our library must therefore be able to present the following elements in a first step:

- An interface with Monte-Carlo codes (MCNP and SERPENT) for criticality, spectrum or local reaction rate calculations - This interface already exists since it was one of the objectives of SMURE.
- A modal decomposition of the Boltzmann equation.
- Some methods to produce diffusion data (on infinite geometries, or fractions of reactors).
- One evolution modules - existing and integrated to SMURE.
- A diffusion solver.
- Some coupling methods with thermohydraulics - partially existing in SMURE.
- A module for the propagation of uncertainties to nuclear data, for static and evolution calculations.

Other IN2P3 projects could lead to new developments of models relevant to reactor physics, such as those developed for multiphysics studies for example (see Pablo Rubiolo's presentation). The library must be built in a flexible way to be able to easily integrate these new models.

i. Definition of a « form »

The possible connection of the different models is essential as soon as one wishes to carry out coupled calculations. Moreover, the production of macroscopic data (diffusion data), whether on a complete geometry or on a geometry of the "infinite" assembly type, must be easily integrated to the NDM calculations or to the evolution calculations on complete cores under the diffusion approximation.

The first step to make our library of models usable is therefore to create a module that allows simple description of core geometries, associated with meshing algorithms adapted to neutronics or thermal-hydraulics solvers. Ideally, each solver, whether neutronic (diffusion, modal decomposition, etc.) or thermal-hydraulic (heat transfer, temperature fields), should be associated with its own mesher in order to optimize the calculations. The transfer of information between the different modules must be easy and easily assimilated to make possible couplings with other models that would not be considered at the present time (such as thermomechanical models).

It is then necessary to build a common "form" that allows to interface all the developed models. SMURE proposes today a philosophy of this type since it is a C++ library whose various classes are called to build the desired simulation. It would be possible to enrich and complete SMURE to offer this role of form for the other developed modules. To do so, many new C++ objects need to be developed, including "super-meshes" for full core calculations in diffusion or modal decompositions.

ii. Benchmark and experimental confrontation

One of the objectives of this numerical framework is to propose easily usable and connectable models whose performances in terms of accuracy and numerical cost are well identified in order to fine-tune the simulations according to the users' needs. Indeed, several numerical methods can

calculate the same observables with different degrees of complexity. For example, at present, the coupling with thermal-hydraulics can be done with BATH or with COBRA-EN. Another example, the evolutions can be carried out on an assembly geometry or a complete core geometry. The difficulty of implementation in both cases is very different.

In order to benefit the contributions of more complex model refinements, it is necessary to quantify these performances by code-to-code comparisons and confrontations with experimental studies. Within our future library, the performances of each model will have to be quantified properly and the results archived.

In this respect, the SPATIAL experimental program (presented by Jean-Luc Lecouey) which consists of a series of measurements of the 3D neutron flux in different transients at the GUINEVERE installation represents a unique opportunity which will allow a large number of kinetic models to be compared. Some of these experiments will be designed to challenge a maximum of existing models in order to improve their validity. For example, we will look for cores strongly coupled with reflectors presenting strong space-energy correlations in order to challenge the point kinetic models but also the Nodal Drift Method.

iii. Data management

This set of models, experiments and benchmarks represents a relatively large amount of information to be archived. The follow-up of knowledge and skills is a crucial issue for us. Today each of the IN2P3 teams develops in a relatively autonomous way without real traceability of the studies (other than by the scientific production and the articles in journals or conferences).

The existence of the SMURE code (and of the CLASS code for cycle physics) allows us to ensure a follow-up of developments. The use of a common git repository so that each one can propose his contributions and the " pear review " of the sources allows to maintain codes and to follow a part of the knowledge, but it happens that some functionalities are not used any more during a few years what necessarily involves a loss of knowledge and know-how.

The definition of an archiving system that should not be too constraining in view of our weak human resources while remaining efficient will mobilize part of our reflections from the first moments of the implementation of this platform. This system could take the form of one (or more) "git repositories" or could be hosted by the CC within the SIREN (SImulation de Réacteurs ElectroNucléaires) group for example.

b. The contribution of the CC-IN2P3 to our activities

The computational needs of such a project can quickly become very important. Currently, we operate very efficiently thanks to the complementarity of local and national computing resources. Thus, each group has a few local machines dedicated to calculations which allows to test the methodologies and to obtain preliminary results on limited configurations. Once the tests have been carried out and the methodologies proven, we can then use the power of the CC-IN2P3 for precision calculations or parametric explorations.

The accessibility to a large number of CPUs in a limited time allowed the realization of numerical models for the calculations of very powerful evolutions. The implementation of this methodology has given IN2P3 a visibility and a privileged place in the international community of cycle physicists that we would not have had without the computing center. We wish to continue to take advantage of this service by using its capabilities to perform Monte-Carlo benchmark calculations but also to build numerical training databases for the different non-linear and multi-parametric regression

methods available. Initially, the aim will be to generalize the use of neural networks for reactor calculations.

i. The importance of HTC for uncertainties and machine learning in reactor physics

To overcome the problem of source convergence in Monte Carlo simulations (see part 1.a), it is possible to perform a large number of identical independent calculations and to make an arithmetic average a posteriori. This proven method is insanely expensive since the variance reduction techniques integrated in MCNP or SERPENT are, by construction, inoperative in this case. Thus, to calculate local reaction rates with a good accuracy, while controlling the statistical uncertainty, it is necessary to perform a very large number of calculations. If it is not possible to consider this approach on a day-to-day basis, it is accessible punctually for specific needs at the CC-IN2P3. Thus, for the benchmarking and characterization of models, it is possible to carry out complete reference core calculations with the stochastic codes at our disposal.

The calculations of uncertainties with the TMC method also require a large number of CPUs in a limited time. The Monte Carlo perturbation theory is expensive in terms of memory as soon as the sensitivity calculations are long to converge. The availability of hundreds of CPUs at the CC offers physicists new ways of dealing with these long calculations. Indeed, on local facilities, a TMC analysis can require several weeks of calculations whereas at the CC the same studies can be performed in half a day. This change of time scale can then allow to consider couplings between TMC calculations and evolution calculations for example or even couplings with parametric exploration approaches like kriging for example.

Finally, the use of CC allowed us to build numerical databases for the construction of neural networks for efficient evolution simulations. The use of these interpolation methods for diffusion is currently being tested and the preliminary results are satisfactory. The generalization of this approach then requires a very important CPU requirement to realize the adequate learning and testing bases. The number of parameters and their types will then be pushed to their maximum in order to push back the limits of the diffusion by refining to the extreme the transport calculations by taking into account parameters neglected until then.

ii. Future needs

Depending on the involvement of the different physicists, the CPU requirements could increase in the next few years, but the quotas allocated to the SIREN group do not really seem to be limiting in the short term. The need for RAM memory per CPU remains problematic today for sensitivity calculations with Monte-Carlo methods, but by dividing a calculation into several independent calculations, there should be no technical impossibility with the means offered by the CC.

Beyond the construction of scattering data and the learning of neural networks, new numerical needs are emerging regularly. For example, modal decomposition requires a high dimensional matrix diagonalization step that can require very large memory resources. The use of GPUs could potentially accelerate the computations but the gain must be quantified, especially in view of the effort required to make our codes compatible.

Finally, the current resources, if they are maintained, will allow us to ensure the major part of the objectives in 5 years. Beyond that, specific needs could arise involving significant memory resources per CPU or GPU calculations, but these are not yet perfectly defined.

c. Fallout of a digital platform and difficulties

As mentioned earlier, such a digital platform would archive our knowledge, simplify the studies of physicists and streamline our research efforts for greater efficiency. Beyond that, the benefits of such a platform are also numerous. First of all, in terms of international visibility with research organizations, the availability of all of our hierarchical models may allow us to gather colleagues from other institutions to this effort. In this respect, the availability of SMURE sources has allowed us to count on several other international developers. It is important to remember that the human resources of IN2P3 are limited and that the maintenance of our codes is not guaranteed in the long term, given the workload that this task requires.

The use of these digital tools within the teaching, whether it is during the training courses at the bachelor or master level, or during the internships or PhD, represents a long-term possible valorization. Indeed, the students who master our tools are able to continue to use them and to promote them during their career. It is in this way that CLASS and SMURE are used in industrial R&D centers.

To initiate this approach, we propose to rely first on the institutional framework related to the development and maintenance of the CLASS and SMURE codes at IN2P3. It is formalized by the Master Project OSCAR, which was launched in 2022, and which is notably centered on the integration in the CLASS and SMURE codes of recent and future advances (within 5 years) that will be carried out in the framework of our research activities. The description of the whole project (objectives and means to achieve them) is described in the IN2P3 project sheet. The following paragraphs summarize in a few lines the relevant actions of OSCAR which allow to initiate the construction of this platform.

For SMURE, the OSCAR project must allow the integration of all the coupled simulation methods (neutronics/thermohydraulics) and the calculations of uncertainty propagation. As explained in this document, the first step is to allow the generation of neutronic scattering quantities over large areas (typically half an assembly) in order to be able to use the available scattering solvers which are necessary for all transient studies. Moreover, the couplings between the different neutronic and thermal-hydraulic solvers exist but are not optimized, nor flexible, making their use restrictive and limited (description of the geometry in Cartesian only and coded "by hand"). The integration of sNDM to SMURE should then allow to answer part of the problems posed by this project (description of the geometry and adapted mesher, production of diffusion data, interface between transport codes and diffusion,...).

As far as the CLASS code is concerned, the previous developments have been largely turned towards the modeling of reactors using advanced mathematical methods (from the Machine Learning theme). These reactor models, which offer new perspectives because of their speed of execution, could greatly enrich the library of our models, but integration into the SMURE environment is currently difficult.

OSCAR should also allow to prepare the integration of other models developed at IN2P3 in the framework of other projects, in particular the modal decomposition or various mutli-physical models. During the OSCAR project, we have to think about the data management and the universal geometries description module.

In the longer term (10 years), the compilation of the different studies associated with the models will have to be integrated into the defined framework. The model-to-model comparisons will then have to be built according to the envisaged domains of validity. The objective is to put this platform into operation within 10 years.

The resources available to do this remain a critical point of this action. If we estimate about one person full time for the exploitation and the maintenance of such a platform, its construction and its implementation require consequent reinforcements. In front of our resources in presence and without reinforcement, that means that certain actions of research will have to be put in second plan to make this project viable.

Conclusion

For more than 25 years, IN2P3 has been involved in reactor physics and fuel cycle physics in order to build an expertise on the future of nuclear power. We have studied the potential of several systems with different degrees of maturity in the thorium and uranium cycles in order to quantify their interest from the point of view of resource economy, waste production and safety. To do this, we have developed innovative methodologies to carry out these studies while seeking to control errors, whether they are due to numerical biases or induced by uncertainties in physical data such as nuclear data. In this respect, several nuclear reactor models have been built, whether for fuel evolution or power transient analysis. All these models are now commonly used for cycle physics studies or reactor design.

The national context of nuclear energy is in constant evolution and the technologies put forward in the public space can be of very different nature. We can distinguish between projects associated with industrialists on existing reactors (such as the replacement of the current French fleet by EPR2s), new types of reactors such as SMRs, and more exotic systems that are very promising on paper but which have many technological barriers that have yet to be overcome. Our academic position, focused on the understanding of the physical phenomena that govern the behavior of neutrons to build an expertise on the modeling of reactors, offers us a place among the actors of French research, complementary to that of the CEA, IRSN or industrial R&D. The study of different systems allows us to explore very vast domains for neutron models while developing a vision on the potential, the relevance and the reality of the different technologies envisaged nationally for the future of nuclear energy.

This dual approach (microscopic modeling of criticality for macroscopic studies of the properties of nuclear systems) has allowed us to develop different unitary (or elementary) models for each of the necessary steps in reactor physics: solving the neutron transport equation, calculating reaction rates and heat deposition, temperature distributions and transient analyses, and material evolution. For each of these models, several resolution methods can be considered depending on the desired accuracy. The fine analysis of the errors, coupled with a multi-system approach, allowed us to build a real expertise on the relevance of the application cases of each solver.

Thus, we were able to determine the situations where the two-level calculation schemes do not give satisfactory results and we quantified the impact on these modeling biases. The impact of assumptions in solving the transport on the production of the diffusion data has been quantified and we are able to propose innovative options to improve the interpolations of the macroscopic cross sections for solving the diffusion equation. Conditions where fuel evolutions must integrate the core physics scale have been identified and explained. New models for cycle studies have been built with DONJON when precision calculations are desired. Finally, several couplings between neutronics and thermal-hydraulics have been studied and are available today in the SMURE environment. All these works allow to propose academic tools for the design of reactors and for prospective studies on the reactors envisaged in the future. The quantification of errors has led us to develop and use innovative propagation methods to test their possibilities. Thus we are now able to prioritize the sources of errors even if they are of very different natures.

Today, we wish to capitalize on this knowledge by gathering all the models built at IN2P3 within a common digital library where each model would be qualified according to the triptych precision, complexity and numerical cost. This library would not only rationalize our development efforts but also strongly enhance IN2P3's know-how and approach. For this library to be relevant, it is necessary that the different elementary digital bricks be easily connectable and interchangeable (when possible). To do this, it is necessary to have a common form that would interface all the external codes with the different internal modules in order to be able to carry out complete studies in reactor physics. Each of these unit models, as well as each complete model integrating a chain of several models, must be compared to international standards. Accuracy and numerical costs must be quantified according to the application cases. In this way, everyone will be able to choose the degree of complexity to be integrated in the reactor simulations, depending on the desired accuracy of the studies.

External references

[Chab, 2020] G. Martin, Ph. Miranda, F. Courtin, and C. Chabert. *Avancement des études de scénarios intégrant les concepts de multi-recyclage rep selon différentes trajectoires d'évolution de la puissance du parc. Gestion des matières (U et Pu) et études de scénarios,* Audition par la Commission Nationale d'Evaluation des recherches et études relatives à la gestion des matières et des déchets radioactifs (CNE2) coordonnée par le Commissariat à l'énergie atomique et aux énergies alternatives du 12 février 2020 (2020).

[Chev, 2016] T. Chevret, *Mesure de la réactivité de réacteurs sous-critiques pilotés par accélérateur par l'analyse d'expériences d'interruptions de faisceau programmées,* thèse de doctorat, université de Caen (2016)

[Dum, 2014] Eric Dumonteil, Fausto Malvagi, Andrea Zoia, Alain Mazzolo, Davide Artusio, et al., *Particle clustering in monte carlo criticality simulations*. Annals of Nuclear Energy, vol. 63, p 612–618 (2014)

[Dum, 2021] Dumonteil, E., Bahran, R., Cutler, T. et al. *Patchy nuclear chain reactions*, Commun Phys 4, 151 (2021)

[Var, 2020] Variansyah I., Betzler B, Martin, William. *Multigroup Constant Calculation with Static α-Eigenvalue Monte Carlo for Time-Dependent Neutron Transport Simulations.* Nuclear science and engineering: the journal of the American Nuclear Society (2020)

[Vit, 2021] Vitali V, Chevallier F, Jinaphanh A, Zoia A, Blaise P. *Comparison of Direct and Adjoint k and α-Eigenfunctions*, Journal of Nuclear Engineering (2021)

[Zoi, 2014] Zoia A., Brun E., Malvagi F, *Alpha eigenvalue calculations with TRIPOLI-4,* Annals of Nuclear Energy, Vol 63 (2014)

Internal references

[Auf, 2015] M Aufiero, A Bidaud, M Hursin, J Leppänen, G Palmiotti, S Pelloni, et al., *A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT,* Annals of Nuclear Energy 85, 245-258 (2015)

[Auf, 2016] M Aufiero, A Bidaud, M Fratoni, *Continuous energy function sensitivity calculation using gpt in monte carlo neutron transport: Application to resonance parameters sensitivity study,* International Congress on Advances in Nuclear Power Plants (ICAPP 2016), 826-830 (2016)

[Bid, 2016] A Bidaud, P Olbratowski, X Doligez, E Autino, M Aufiero, B Leniau, *Understanding Total Monte Carlo uncertainty propagation in burn up calculations with Generalized Perturbation Theory,* International Conference on Nuclear Data for Science and Technology (ND2016)

[Cap, 2009] N Capellan, A Bidaud, S David, O Meplan, A Nuttin, J Wilson, J Brizi, zet al. *3D coupling of Monte Carlo neutronics and thermal-hydraulics/thermic calculations as a simulation tool for innovative reactor concepts,* International Conference GLOBAL 2009, Paris (2009)

[Cou, 2017] F Courtin, B Leniau, N Thiollière, B Mouginot, X Doligez, A Somaini, *Neutronic predictors for PWR fuelled with multi-recycled plutonium and applications with the fuel cycle simulation tool CLASS,* Progress in Nuclear Energy 100, 33-47 (2017)

[Ern 2015] M Ernoult, S David, X Doligez, O Meplan, B Leniau, A Bidaud, A Nuttin, et al,.*Advanced plutonium management in PWR, complementarity of thorium and uranium,* Progress in Nuclear Energy 78, 330-340 (2015)

[Ern, 2019] M Ernoult, X Doligez, N Thiollière, AA Zakari-Issoufou, A Bidaud, et al. *Global and flexible models for Sodium-cooled Fast Reactors in fuel cycle simulations,* Annals of Nuclear Energy 128, 69-76 (2019)

[Ern, 2021] M. Ernoult, J. Liang, X. Doligez, N. Thiollière, O. Méplan, et al., *Automated selection of nuclides and reactions of interest in a depletion simulation. Precision loss estimation for multiple outputs,* Progress in Nuclear Energy, Volume 135 (2021)

[Gui, 2021] M. Guillet, X. Doligez, G.Marleau, M. Paradis, M. Ernoult, N. Thiollière, *Coupled CLASS and DONJON5 3D full-core calculations and comparison with the neural network approach for fuel cycles involving MOX fueled PWRs*, Annals of Nuclear Energy, Volume 152 (2021)

[Len, 2015] B Leniau, B Mouginot, N Thiolliere, X Doligez, A Bidaud, F Courtin, et al., *A neural network approach for burn-up calculation and its application to the dynamic fuel cycle code CLASS,* Annals of Nuclear Energy 81, 125-133 (2015)

[Mep] O Méplan, J Hajnrych, A Bidaud, S David, N Capellan, B Leniau, A Nuttin, et al. *MURE 2: SMURE, Serpent-MCNP Utility for Reactor Evolution User Guide, L*aboratoire de Physique Subatomique et de Cosmologie

[Mou, 2014] B Mouginot, B Leniau, N Thiollière, M Ernoult, S David, X Doligez, et al. *Core library for advanced scenario simulation, CLASS: principle & application,* International Conference PHYSOR 2014 (2014)

[Nut, 2012] A Nuttin, P Guillemin, A Bidaud, N Capellan, R Chambon, S David, et al. *Comparative analysis of high conversion achievable in thorium-fueled slightly modified CANDU and PWR reactors,* Annals of Nuclear Energy 40 (1), 171-189 (2012)

[Nut, 2013] Nuttin, A., Capellan, N. et al., *Facing Challenges for Monte Carlo Analysis of Full PWR Cor*es, Proc. Int. Conf. SNA+MC 2013.

[Nut, 2016] Nuttin, A., Prévot, P. et al., *Validation of the minimalistic Nodal Drift Method for spatial kinetics on a simple CANDU LOCA benchmark*, Annals of Nuclear Energy, 88, 135-150 (2016).

[Par, 2019] E. Party, X. Doligez, P. Dessagne, M. Kerveno, G. Henning,, *Uncertainty quantification and sensitivity studies on Thorium-fueled reactors,* EPJ Web Conf. Volume 239, 2020 (ND 2019)

[Par, 2021] M. Paradis, X. Doligez, G. Marleau et al. *DONJON5/CLASS coupled simulations of MOX/UO2 heterogeneous PWR*, EPJ Nuclear Sci. Technol., Volume 7, (2021)

[Pre, 2017] Prévot, P., Nuttin, A. et al., *Enhancements to the Nodal Drift Method for a Rod Ejection Accident in a PWR-like mini-core with lumped thermal model*, Annals of Nuclear Energy, 101, 128–138 (2017).

[Pre, 2017] Prévot, P., Nuttin, A. et al., *Preliminary Design Studies by a Complete Academic Simulation Toolbox of a Water-Cooled Thorium-Fueled Small Modular Reactor Core*, Proc. Int. Conf. GLOBAL (2017).

[Sab, 2014] P Sabouri, A Bidaud, S Dabiran, D Lecarpentier, F Ferragut, et al. *Propagation of nuclear data uncertainties in deterministic calculations: application of generalized perturbation theory and the total monte carlo method to a PWR burnup pin-cell,* Nuclear Data Sheets 118, 523-526 (2014)

[Som, 2016]A Somaini, S David, X Doligez, AA Zakari-Issoufou, A Bidaud, et al., *The impact of reactor model simplification for fuel evolution: a bias quantification for fuel cycle dynamic simulations,* International Congress on Advances in Nuclear Power Plants (ICAPP 2016)

[Til, 2019] L. Tillard, J.B. Clavel, X. Doligez, E. Dumonteil, M. Ernoult, J. Liang, *Development of a multi-zone irradiation model for scenario studies involving ASTRID like SFRs*, ICAPP 2019, France (2019)

[Thio, 2015] Thiollière N., Courtin F., Leniau B., Mouginot B., Doligez X., Bidaud A., *Prediction of MgO volume fraction in an ADS fresh fuel for the scenario code CLASS,* Progress in Nuclear Energy Vol. 85, p518-524 (2015)

[Zak, 2017] AA Zakari-Issoufou, X Doligez, A Somaini, Q Hoarau, S David, S Bouneau, et al. *Americium mono-recycling in PWR: A step towards transmutation,* Annals of Nuclear Energy 102, 220-230 (2017)

Annexe 1 : Thèses soutenues et en cours

Soutenues :

Franco Michel Sendis (2006) : Contribution à l'étude de la production d'233U en combustible MOX-ThPu en réacteur à eau sous pression : application aux scénarios de transition vers des concepts isogénérateurs Th/233U en spectre thermique : développement du code MURE d'évolution du combustible

Perrine Guillemin (2009) : Recherche de la haute conversion en cycle thorium dans les réacteurs CANDU et REP : Développement des méthodes de simulation associées et étude de scénarios symbiotiques

Nicolas Capellan (2009) : Couplage 3D neutronique thermo hydraulique : développement d'outils pour les études de sûreté des réacteurs innovants

Julie Brizi (2010) : Cycles uranium et thorium en réacteurs à neutrons rapides refroidis au sodium : Aspects neutroniques et déchets associés

Robert Sogbadji (2012) : Neutronic study of the mono-recycling of americium in PWR and of the core conversion INMNSR using the MURE code

Jean-Baptiste Clavel (2012) : Etude de systèmes et scénarios électronucléaires double strate de transmutation des actinides mineurs en ADS

Van minh Bui (2012) : La décroissance bétâ des produits de fission pour la non-prolifération et la puissance résiduelle des réacteurs nucléaires

Baptiste Leniau (2013) : Caractérisation des sources radioactives du cycle du combustible. Applications au cycle du thorium : synthèse de l'232U en combustibles solides

Pouya Sabouri (2013) : Application of perturbation theory methods to nuclear data uncertainty propagation using the collision probability method

Sandrine Cormon (2013) : Etude du potentiel de la détection des antineutrinos pour la surveillance des réacteurs nucléaires à des fins de lutte contre la prolifération.

Anthony Onillon (2014) : Prédiction des taux de fission des cœurs de Chooz et estimation des incertitudes associées dans le cadre de l'expérience Double Chooz

Marc Ernoult (2014) : Gestion avancée du Plutonium en REP Complémentarité des cycles thorium et uranium

Alice Somaini (2017) : Analyse des erreurs induites par une modélisation simplifiée sur l'évolution des combustibles REP Impact des fuites neutroniques dans les calculs cellules

Fanny Courtin (2017) : Etude de l'incinération du plutonium en REP MOX sur support d'uranium enrichi avec le code de simulation dynamique du cycle CLASS

Pierre Prévot (2018) : Développement d'outils académiques pour la conception et la sûreté de réacteurs innovants : premières applications au dimensionnement de SMR refroidis à l'eau légère et chargés en thorium

Lea Tillard (2019) : Impact du déploiement de réacteurs de type ASTRID sur la gestion dynamique du plutonium dans des scénarios de transitions électronucléaires

Eliot Party (2019) : Etude des réactions (n, xn) pour les noyaux fertiles / fissiles du cycle du combustible innovant au Thorium

Pamela Lopez (2021) : Méthodes de dimensionnement des incertitudes d'une chaine industrielle de calcul cœur

En cours :

Davide Portinari (2022) : SYBIL: Incertitudes en évolution

Adrien Rispo (2023) : Modélisation de la remontée de flux axiale dans les réacteurs REP

Yohannes Molla (2024) : Quantification des incertitudes et analyses de sensibilité pour la puissance résiduelle. Impact des données nucléaires.

Annexe 2 : Principales collaborations

Projets NEEDS

Nous collaborons avec les autres acteurs de la recherche au niveau national dans le cadre de projets NEEDS. Actuellement, les activités sur les incertitudes sont coordonnées dans le projet structurant SUDEC, coordonné par Adrien Bidaud, qui regroupe l'IRSN, le CEA et l'IN2P3. Le projet structurant CINEASTE, coordonné par Nicolas Thiollière et qui propose une réflexion interdisciplinaire sur les scénarios nucléaires (voir contribution de Marc Ernoult), comporte un axe fort sur la modélisation des réacteurs nucléaires en évolution. Le partenaire privilégié sur cet axe est le CEA. Les

recherches sur l'utilisation du machine learning pour la production et l'utilisation des données de diffusion sont réalisées en collaboration avec l'IRSN (et l'école polytechnique de Montréal) au sein du projet MADIFF.

Enfin, l'ensemble des travaux sur les incertitudes aux données nucléaires sont liés au projet structurant NEEDS NACRE (voir la contribution de Maëlle Kerveno).

Industriels

Actuellement, des collaborations étroites et bilatérales existent sur des questions précises. Ces projets sont souvent limités dans le temps, mais les échanges informels s'étalent souvent au-delà des contrats de collaboration. Ainsi, on peut noter que 3 thèses en cours sont liés à des collaborations bilatérales :

- La thèse de Pamela Lopez est une collaboration avec EDF sur les incertitudes et l'assimilation des données dans les chaines de calculs industrielles
- La thèse de Davide Portinari s'insère dans le cadre d'une collaboration avec Technicatome sur les incertitudes en évolutions (notamment auprès du réacteur ILL dans le cadre de la thèse, mais au-delà sur d'autres actions de la collaboration).
- La thèse d'Adrien Rispo est une thèse CIFFRE sur la problématique des remontées de flux à l'interface axiale cœur/réflecteur

Collaborations académiques internationales

Par le passé, plusieurs collaborations avec des laboratoires américains ont eu lieu. En 2022, nous pouvons noter la collaboration avec l'Institut de Génie Nucléaire de l'école polytechnique de Montréal qui permet le co-encadrement d'étudiant depuis 2015 environ (3 étudiants à ce jour). L'IGN développe et maintien la chaine DRAGON/DONJON, l'unique chaine déterministe académique et libre d'utilisation disponible dans le monde.

Au sein de la NEA, Subatech participe au groupe WPNCS (Working Party on Nuclear Criticality Safety) SG10 on nuclear data uncertainties propagation on spent fuel inventory de la NEA