The APOLLO3® scientific tool for SFR neutronic characterization: current achievements and perspectives

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Abstract.

ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration) is a Sodium Fast Reactor design that will be France's Flagship 4th Generation Reactor.

Its innovative core contains many axial and radial heterogeneities (in order to obtain a negative void coefficient) and interfaces that are challenging for current deterministic codes to simulate correctly. Hence there is the need for new improvements in modeling (3D simulations, parallel processing) like those being elaborated within the APOLLO® platform.

The APOLLO3-SFR package built with APOLLO3® solvers defines reference calculation schemes associated with a nuclear data library to calculate all neutronic parameters (critical masses, sodium void, Doppler coefficient, βeff, etc…) together with certified biases and uncertainties derived from the VV&UQ process. This VV&UQ process incorporates numerical validation, a-priori uncertainties based on nuclear data covariances as well as experimental validation mainly from MASURCA, a fast mock-up reactor, located at CEA Cadarache. A future programme called GENESIS will be performed in support to the prototype ASTRID to validate the CFV core specificities. In addition, a part of the GENESIS experimental program contains integral experiment underway at the BFS facility.

The paper presents the APOLLO3-SFR neutronic platform latest development and the various VV&QU activities which are currently conducted to derive all neutronic characteristics with a certified uncertainty.

Key Words: APOLLO3®, ASTRID, VV&UQ, Integral experiment

1. Introduction

Even though Sodium Fast Reactors (SFR) have acquired years of experience, designing future SFR reactors requires however to enhance their operational performance and reduce the probability to go into core disruption. ASTRID, one of these novel reactors has a rather large core with a flat shape, to reduce significantly the Sodium Void Effect (SVE) [1]. Hence there is the need for new improvements in modeling (3D simulations, parallel processing) like those being elaborated within the APOLLO3® platform.

The novel platform APOLLO3® is facilitated by the advances of modern languages like C ++ and numerical methods but also new computing resources both by increasing the number of operations per second and the volume of data storage. This platform is designed to meet the new needs of current core designs and the associated uncertainty reduction requirements. This concerns primarily the prototype ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration).

The functionalities available in APOLLO3® [2] will ultimately lead to a single reference calculation scheme regardless of the type of reactor core. The physical characteristics of SFR

have required specific solver developments to meet target accuracy, in particular all aspects related to neutron leakage treatment. The implementation of such solver developments yield improved results for SFR cores but also for more traditional core concepts either fast or thermal.

To build on safety records, the APOLLO3® calculation scheme requires a VVUQ process (Verification, Validation and Uncertainty Quantification) to deliver not only improved results but proof of its performance and reduced uncertainties.

The objectives of VV&UQ process applied to ASTRID is to provide a validated (i.e. reliable) neutronic code package, checked on experiments with reduced uncertainties lower than the target accuracy. This code package is called APOLLO3-SFR, built on the APOLLO3® generic platform [3]. Chapter 2 presents the ASTRID core: the so-called Low Void Core (CFV in French) and its physical specificities. Chapter 3 describes the choice of solvers, algorithms and associated approximations in relation to SFR specificities and particularly those of the CFV core. Chapter 4 presents the basic philosophy behind the VV&UQ approach applied to the CFV core of ASTRID and details each part of this process with a short description of the physics involved (Nuclear data, Transport code and integral experiments). Ultimately, the GENESIS experiments in support of the final uncertainty quantification is being reviewed and illustrated.

2. ASTRID Basic Design and Major Neutronic Parameters

2.1. SFR Generic Neutronic Requirements

The APOLLO3® code system must be able to meet the generic specifications of fast neutron reactor cores such as the ones of PHENIX and SUPER-PHENIX:

1. The precise representation of threshold fission reactions such as U238, Pu240 or Am241.

2. The treatment of the inelastic slowdown which includes discrete levels and resonances. The inelastic cross-section of Iron requires, for example, the self-shielding calculation.

3. The treatment of the elastic slowing down of "light" elements (Oxygen, Sodium, Fe, for example) in fast reactors requires a fine energy description at many groups, essentially between 100 eV and 5 MeV.

4. The inelastic and elastic collision anisotropy is a non-negligible effect. The anisotropy increases at high energy even for elastic and important variations occurs in the oxygen resonance at 440 keV whose average cosine of deviation due to the anisotropy of the collision changes sign in the middle of the resonance. This effect is treated by means of P0 and P1 matrices, sufficiently detailed in energy and separated according to the reactions.

5. The cross-section self-shielding in the 100 keV -1 keV energy domain, zone of unresolved resonances, is important. The approximation of the narrow resonances is well justified in this energy domain and allows a simplification of the calculations with a very significant reduction of the calculation times.

6. Fast reactor cores require a precise self-shielding without making assumptions on the neutron slowing down process. The self-shielding of heavy isotopes located in zones of very different compositions requires the subgroup method.

7. The very important neutron leakage requires specific treatment (streaming) at the sub-assembly level and at the core level.

8. The sub-assembly geometries for fast reactors exhibit a series of pins on a hexagonal pattern enclosed by a steel wrapper. These require precise algorithms either exact collision probabilities or MOC (method of characteristics) with features allowing fundamental mode treatment (heterogeneous neutron leakage).

9. Fast neutron reactors cores require the use of the transport theory for describing correctly the power map distribution (about 5% of bias induced for SUPER-PHENIX by the use of the diffusion theory), the control rod reactivity (about 10% for SUPER-PHENIX) and the reflector gains (a few hundred pcm on the reactivity and flux distortions at the interface). On a benchmark of the BN1800 core with a sodium plenum, the sodium void reactivity is increased by 2$ due to transport effect.

10. The spatial codes must be able to describe XYZ geometries which are those of most integral experiments and Hex-Z geometries which are those of the reactor cores.

These features have led to the solver main choices of APOLLO3-SFR, with a 1968 group library exhibiting probability tables, P3 scattering matrices separated into elastic, inelastic and n,xn reactions.

2.2. ASTRID core description

Designing a Sodium Fast Reactor Core is associated to many criteria very much linked to neutronic characteristics such as breeding gain (sustainable nuclear energy –more than 100 times those using only PWRs), fissile inventory (economy), reactivity coefficients associated to Dynamic Feedback Coefficients (plant inherent behaviour; grace time), reactivity effects associated to accidental initiators (safety), reflectors or dirty blankets (Non-proliferation), reduction of waste radiotoxicity (Public Acceptance).

The ASTRID core [1] aims at answering such objectives. The core combines many geometric features (fertile, plenum sodium, absorbing plate, reduced core height configuration) leading to a negative void reactivity coefficient (-$0.5 at the end of the Fuel Cycle) without degrading core performances. The RZ core description presented on Figure 1 illustrates such specificities.

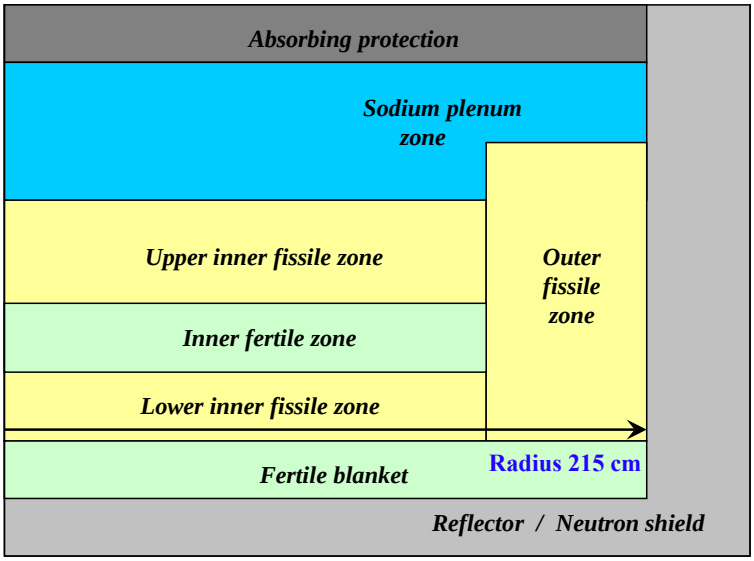

Figure 1. Section of the ASTRID core (1500 MWth)

2.3. Neutronic challenges in the ASTRID core design

The ASTRID CFV core contains specific features that require the development of innovative calculation schemes.

1. The Sodium Plenum

The sodium plenum, once voided, leads to important empty zones that require transport codes such as Sn codes. The presence of the hexagonal tube and the end-plugs of the fissile pins require specific treatments at the sub-assembly level (3D MOC).

2. The internal fertile plate

The internal fertile plate requires a 3D self-shielding particularly for taking heterogeneity into account. These problems are exacerbated in a voided situation.

3. The core / reflector interface

The steel reflectors requires a fine group treatment of the reflective gain as neutrons are scattered on the iron broad resonances which have the double role of slowing down neutrons and moving them back into the core at lower energy.

4. The treatment of heterogeneous control rods

The preparation of the cross sections of the heterogeneous bars requires a particular treatment linked to the very strong coupling of the heterogeneous flux structure in the control rods to that of the one of the surrounding core cells. Solvers using non-conforming or unstructured meshes would allow a better representation of the geometries of these control rods in their environment.

5. The calculation of certain parameters such as the fraction of delayed neutrons βeff and the lifetime of fast and delayed neutrons,

6. The calculation of the global feedback coefficients by geometry subdomains. The peculiarities of the ASTRID geometry require 3D HexZ perturbation calculations in transport theory.

In conclusion, generic requirements for Fast Reactor cores and those specific to the new ASTRID cores require new solvers capabilities to meet increased safety requirements.

3. APOLLO3-SFR reference calculation scheme

The typical calculation scheme for APOLLO3® is presented in Figure 2. It is based on the separation of the sub-assembly calculation (orange) from the core calculation (green).

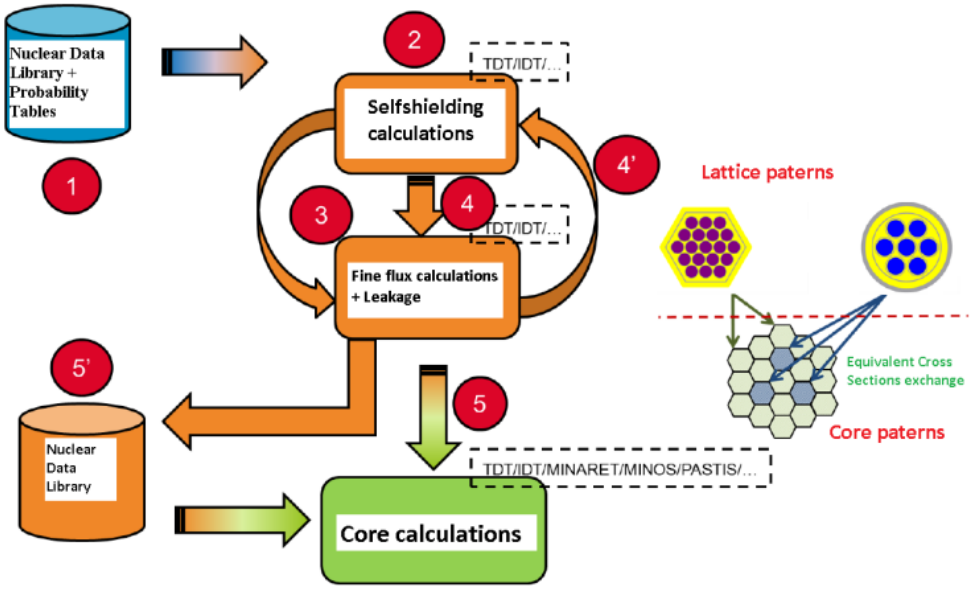

Figure 2: APOLLO3® calculation scheme

First, the code sets the nuclear data multi-group libraries, associated with probability tables, following the energy grid choice by the user (1). Then occurs the self-shielding (2), which generates self-shielded cross sections of relevant resonant isotopes in different regions. Those cross sections are used in the sub-assembly flux calculation (3), and this process repeats itself (4) with an update of the fission and slowing-down sources. In the end, we obtain self-shielded cross sections which are condensed, homogenized (5 & 5') and stored in a Multi-Parametric Output library (MPO). Finally, we use different sub-assemblies MPOs to launch the core calculation.

In order to achieve the required accuracy for designing the ASTRID core and based on the physical analyses of SFR cores in general and CFV core of ASTRID in particular, the choice of the APOLLO3-SFR reference calculation scheme [4] has been done in this way:

1. The 1968 group structure of ECCO [5] is chosen on the basis that the self-shielding methods are insufficient if the resonances are wide or intermediate and only the narrow resonance approximation is accurate enough. The choice of the group scheme is therefore made on the basis of the slowing of the neutron on a heavy isotope (in this case the U238) with assumptions: elastic and isotropic collision on the U238.

   The fraction (in %) of the neutrons which remain in the group for groups with constant lethargy is already important in a 1/120 energy grip scheme (Table 1).

Table 1 : Fraction of neutrons remaining in the group

Δu	%
1/480	6.243
1/240	12.487
1/120	24.875

   The use of the library at 3586 groups (1/480 in lethargy for most of the groups) [6] has shown a rather small improvement but associated with an increase in the running time

of about 2. The evaluated nuclear data library is processed with the GALILEE [7] system to produce multi-group cross-sections set in a 1968 groups structure for all isotopes with distinctions between elastic, inelastic and (n,xn) transfer matrices. Those matrices are described up to P5 Legendre order expansion.

2. Resonances are represented by probability tables when included in the group and are used by the subgroup method. The probability tables of resonant isotopes are processed with the CALENDF code (module of GALILEE). The subgroup method calculates self-shielded cross-sections using the Narrow Resonance approximations and usual hypotheses associated to the collision probability method (flat flux in each region, integration over angle). Collision probabilities are calculated with the TDT-CPM solver (exact Pij).
3. Since the collision probability assumptions are not acceptable at the flux sub-assembly level (1968 groups), the calculation is performed with the method of characteristics using the TDT-MOC solver [8]. The B1 heterogeneous algorithms [9] have been implemented in order to better represent neutron leakage. The geometry modelled by TDT-MOC is the same than the one of TDT-CPM but the tracking parameters of TDT-CPM are less refined than TDT-MOC ones. The symmetry properties of the sub-assemblies (description of only 1/12th of the full sub-assembly) (Figure 3) are used to save running times. Fuel sub-assemblies are described with reflective boundary conditions. This TDT-MOC flux solver is coupled with the subgroup method using the TDT-CPM solver (exact Pij) with the same geometry.

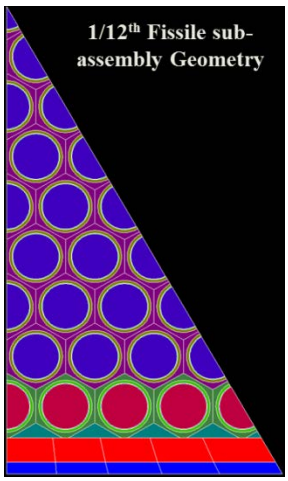

Figure 3: 1/12th Fissile sub-assembly Geometry

4. The sub-critical sub-assemblies (fertile, control rod and structural media) are modeled by clusters [4] i.e. geometries at the center of which the sub-critical sub-assembly is located and surrounded by a ring of fuel sub-assemblies. Again, the symmetry properties of the sub-assemblies (description of only 1/12th of the full sub-assembly) (Figure 4) are used to save running times.

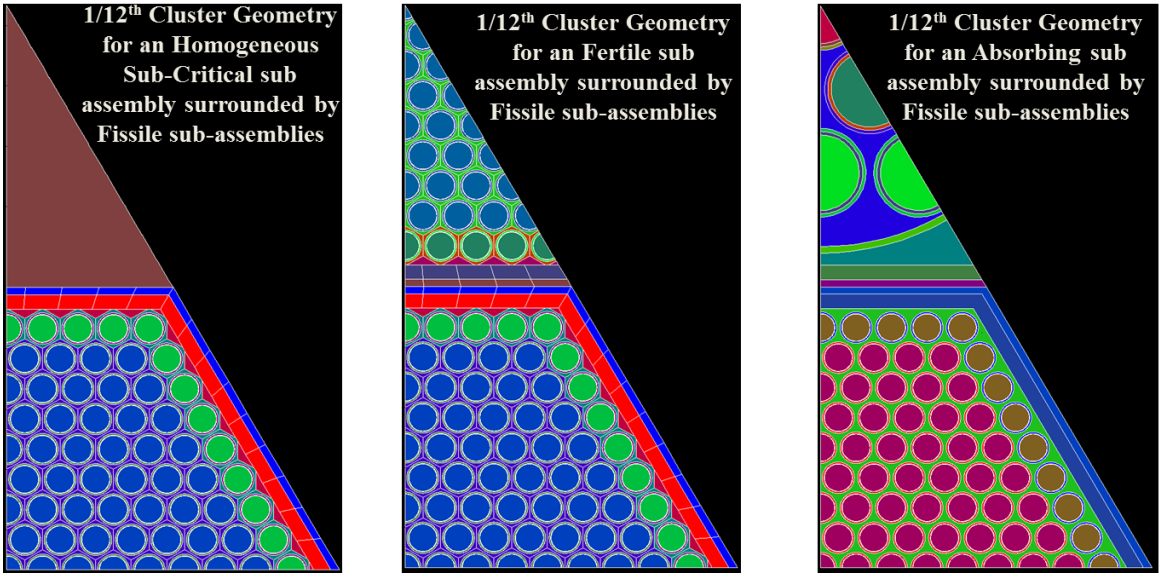

Figure 4: 1/12th Fissile sub-assembly Geometry

5. The TDT-MOC flux solver iterates with the subgroup method using the TDT-CPM solver (exact Pij) until convergence is reached. Then, the self-shielded cross-sections are collapsed in a larger energy group scheme (typically, 33 groups) and smeared either completely (fuel sub-assemblies) or partially (for the central sub-critical sub-assemblies). The moments of the flux coming out from the B1 heterogeneous leakage treatment allow a group condensation and a smearing which preserves the neutron balance without the use of any equivalence method.
6. Finally, the collapsed and homogenized cross-sections are stored in a Multi-Parametric Output library (MPO) for use in core calculations. Core calculations are performed with the 3D Sn core solver MINARET. The MINARET core solver [10] uses an unstructured conforming triangular spatial mesh (Discontinuous Galerkin Finite Elements), which allows the solver to handle any type of geometry. The hexagonal periodicities specific to fast reactors cores, or even cores without real periodicity can be modelled.
7. The specific features of MINARET Sn core solver allow a spatial domain decomposition method (DDM) [11]. Using massive parallelism, DDM allows much more ambitious computations in terms of both memory requirements and calculation time. For current computer capabilities, this is used for a 3D core model of the CFV-kind in which the control rod heterogeneity is kept, while fuel assemblies are homogenized. Doing so, traditional difficulties of core codes to correctly model control rods are overcome.

4. VV&UQ

4.1. General VV&UQ philosophy used

The APOLLO3-SFR package built with APOLLO3® solvers defines reference calculation schemes associated to a nuclear data library for calculating all neutronic parameters (critical masses, sodium void, Doppler coefficient, βeff, etc…) together with certified biases and uncertainties derived from the VV&UQ process.

The ***Verification*** step consists in verifying that numerical resolution of neutronics models and programming of each module of the code package are correct keeping a non-regression policy.

The ***Validation*** *steps are separated in:*

- *Numerical* ***Validation*** step which aims at quantifying the accuracy of the neutronic calculation schemes with APOLLO3® code [12, 13] by comparison to TRIPOLI4® continuous-energy Monte Carlo calculation [14] with the same nuclear data library (JEFF). The reference calculation scheme (smallest numerical biases) and project calculation scheme (to be used on a regular basis for conceptual studies) are defined in an iterative way within this activity.
- Experimental ***Validation*** step (also called "Qualification") corresponds to the comparison of the results of the global package (code + calculation scheme + nuclear data library) against experimental results from integral measurements.

The ***Uncertainty Quantification*** (***UQ***) is the ultimate step. This phase uses experimental results mainly from MASURCA, a fast mock-up reactor, located at CEA Cadarache. A future programme called GENESIS will be performed in support to the prototype ASTRID. In addition, a part of the GENESIS experimental program contains integral experiment underway at the BFS facility. Figure 5 illustrates the VV&UQ methodology used for APOLLO3-SFR.

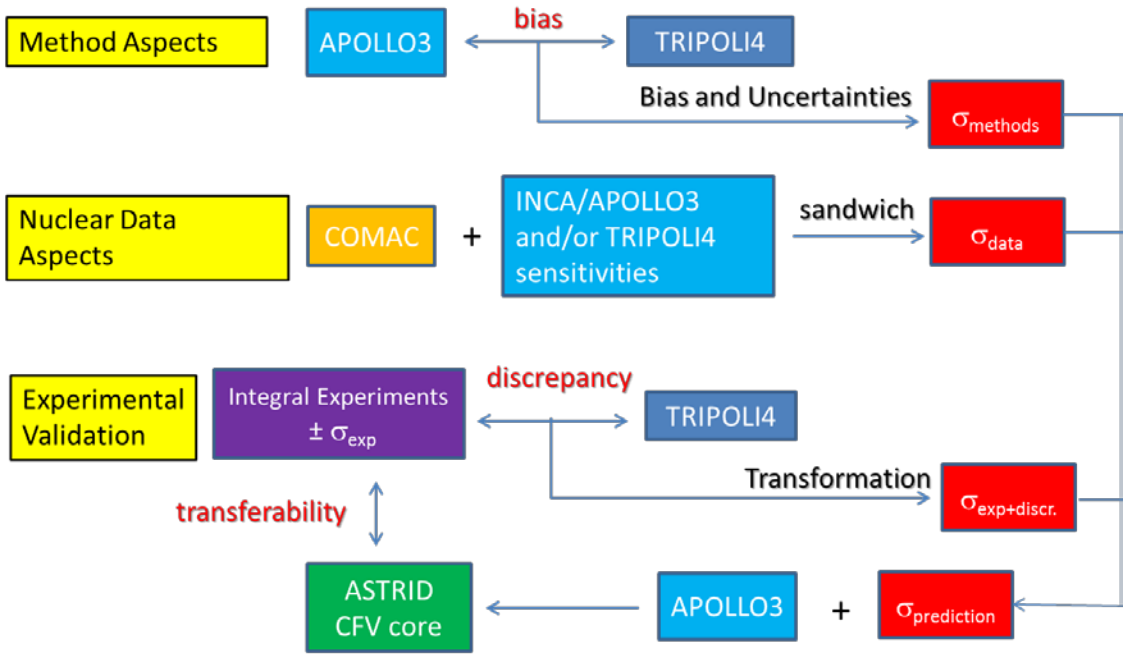

Figure 5. Bias and Uncertainties derived from the VV&UQ process

Thus, APOLLO3-SFR package provides calculation schemes, nuclear data library and a proper list of obtained biases and uncertainties derived from the VV&UQ process.

4.2. APOLLO3® code V&V

Despite technological improvements in computer science (number of operations per second and storage volume increased), approximations are unavoidable in deterministic codes. Yet, those approximations bring more or less important discrepancies on different core characteristics against reference calculations (for example Monte-Carlo). The V&V process is therefore the search of an optimum on these discrepancies between calculation time and accuracy. Since the comparison is done using the same nuclear data library, methods and modelling are the only sources of bias. In previous V&V processes, the estimated bias was the global one, i.e. without identifying the impact of each individual approximation.

The new V&V methodology enables an estimate of biases related to each of the approximations. First, it is important to identify the main approximations involved in the APOLLO3® reference calculation scheme. Then, estimation of biases is performed by comparison of APOLLO3® results with well-chosen reference results (often multigroup Monte-Carlo results). Finally, the advantage of this methodology is illustrated on different SFR core characteristics using the APOLLO3® calculation scheme.

The following table presents the reference APOLLO3® calculation scheme for SFR [4].

Table 2: APOLLO3®-SFR Calculation Scheme

Calculation Step	Functionality	Value
Sub-assembly Calculation	Scattering Anisotropy	P1
	Fission Spectrum incident energy macrogroup	4
	Energy Grid	1968 Groups
	Self-shielding	Sub-group method
	Flux Solver	TDT-MOC (Method of Characteristics)
	Leakage Treatment	B1 Heterogeneous
Core Calculation	Energy Grid	33 Groups
	Flux Solver	MINARET (S_N)

Approximations are directly linked to the functionalities of the code. For example, energy discretization is an approximation which can be estimated by comparison with the continuous-energy TRIPOLI-4® results. The two step calculation (Sub-assembly then Core), combined with the fundamental mode for sub-assembly calculation leads to another approximation which has to be taken into account.

The APOLLO3® generic V&V is meant to validate a large set of neutronic solvers (Pn, Sn, Pij, MOC…) as well as physical functionalities (self-shielding calculations). It is based on the use of a complete validation grid which ensures maximum coverage of the solvers and functionality for standard neutronic physics. This validation is mainly numeric by comparison with reference methods (Monte Carlo and deterministic) [15]. For APOLLO3-SFR package, this V&V activity is then used as guideline for the calculation scheme.

This validation has been conducted first for the core 1 and core 2 sub-assemblies without leakage as seen on the Table 3.

Table 3 : Reactivity Bias split over different approximations

	Reactivity Bias (pcm)	
Assembly	Core 1	Core 2
Global	+ 10	+ 17
Self-Shielding	+ 14	+36
Nuclear Data Treatment	- 1	- 11
TDT-MOC	- 2	- 7

It shows no significant bias and compensating effects are very limited.

However, when leakage is present i.e. when calculating core balance, the discrepancies increase as seen on Table 4.

Table 4 : Reactivity Bias for the core calculation

	Reactivity Biais (pcm)	
Situation	**Nominal**	**Rod inserted**
Global	**+ 154**	**+ 188**

A breakdown of these discrepancies shows that the major source of discrepancy comes from radial steel reflectors. More energy groups are required to treat adequately the neutron slowing down in the resonating iron reflectors and their return to the core at lower energies. More work is on-going to improve the computational scheme for this particular aspect.

4.3. Nuclear data covariances: COMAC-V1

COMAC V1 [16] is the covariance file based on JEFF3.2 [17] evaluation processes. It uses nuclear models and differential measurements.

The propagation of these uncertainties to the ASTRID core characteristics is performed using $S(p,\sigma)$ the sensitivity vector of the neutronic core characteristic p to nuclear data and M_σ the covariance matrix. The relative uncertainty of the core characteristic p due to nuclear data is computed with the following expression: $\varepsilon_p = \sqrt{{}^t S(p,\sigma)\cdot \mathbf{M}_\sigma \cdot S(p,\sigma)}$

In the following table 5, the a-priori ASTRID core characteristics uncertainties due to Nuclear Data are calculated.

Table 5. ASTRID core characteristics uncertainties due to Nuclear Data

ASTRID core characteristic	**Nuclear Data Uncertainties (1σ) (COMAC-V1)**
keff (pcm)	**804**
Sodium Void ($)	0.28
β_{eff}	3.4%
Doppler Effect	2.7%
Rod Worth	2.5%
Ratio P_{max}/P_{tot}	2.5%

Nuclear data uncertainty breakdown contributions identify ^{238}U and ^{239}Pu isotopes as major contributors even for sodium void reactivity effects.

4.4. Integral experiments for APOLLO3-SFR Validation

4.4.1. General Uncertainty flow from nuclear data to neutronic parameters

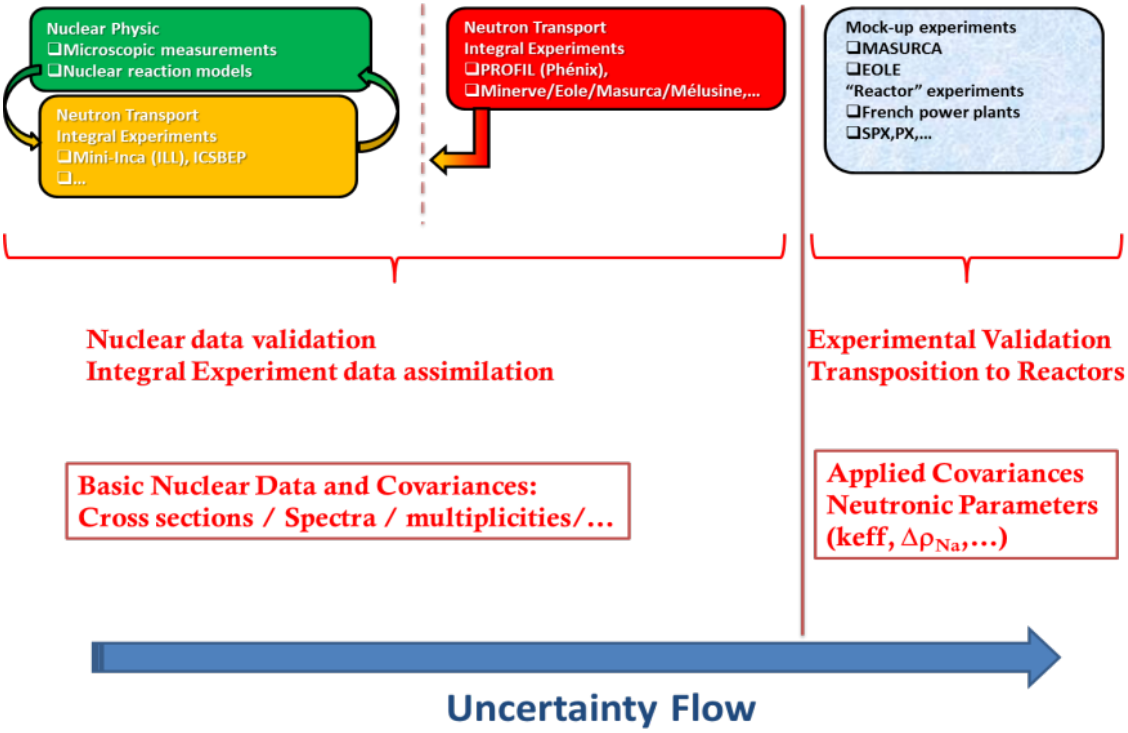

Figure 6. Uncertainty flow from basic nuclear data to neutronic parameters

Figure 6 shows how integral experiments are used for a nuclear data uncertainty reduction [18]. From the a-priori nuclear data uncertainties, use generic zero power integral experiments to reduce the nuclear data uncertainties. Then, dedicated or specific experiments are used to

- quantify the uncertainties of ASTRID CFV core characteristics such as βeff [19] and Doppler.

- quantify the bias and uncertainties of ASTRID CFV core specific characteristics such as sodium void reactivity, control rods or power tilts using BFS experiments (Phases I and III in BFS-2 and Phases II and IV in BFS-1) [20] and MASURCA (GENESIS program).

4.4.2.Nuclear Data V&V

JEFF3.2 nuclear data evaluations were released by NEA in March, 2014. New evaluations for actinides, such as ^{235,238}U, ^{239,240}Pu and ^{241}Am as well a new sodium evaluation are included. To validate such new files, a set of public integral benchmarks (for thermal, intermediate and fast spectrum) were used in the framework of the JEFF project [17]. In addition, CEA's fast reactors integral experiments were used directly for ASTRID nuclear data validation purposes.

Table 6. Critical Mass Integral experiments

MASURCA Experiment	**JEFF3.2 C-E (pcm)**
RACINE-1D B4C	143
RACINE-1D NA	-31
PRERACINE-1	377
PRERACINE-2A	140
PRERACINE-2B	67
ZONA-2A	-66
ZONA-2B	58

For critical masses experiments, JEFF3.2 shows improved results compared to previous evaluation sets mainly due to sodium cross sections and to a better connection between resonance and higher energy ranges for ^{239}Pu.

4.4.3.Nuclear Data V&V

ASTRID core design exhibits very innovative features compared to past reactors (such as Super-Phénix). The ASTRID core is very heterogeneous and achieves negative sodium void reactivity effect through the existence of a large leakage component (Table 7).

Table 7. Break down of Void Effect in the ASTRID CFV core

Component	Void Effect	Central Component	Leakage component
$\Delta\rho_{Na}$ (pcm,$)	-732 (-1.9 $)	879 (2.3$)	-1611 (-4.3$)

The leakage component [21] introduces a change of the fission sources which is significant (Figure 7) especially in the upper and lower parts of the core region.

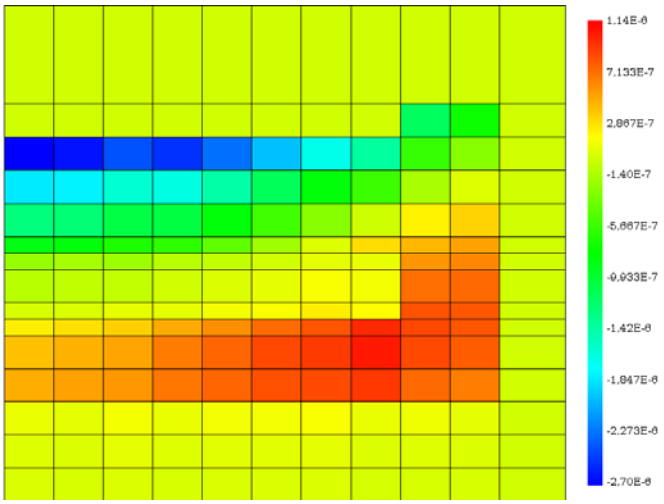

Figure 7. Absolute difference between reference and void volumic fission sources for the leakage component

Hence, there is a real necessity to have dedicated sodium void integral experiments that are close to ASTRID core design. The GENESIS programme in support of these ASTRID core innovative features is currently underway in the BFS facility [20] and will be followed in MASURCA after its refurbishment is completed.

5. CONCLUSIONS AND CHALLENGES

ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration) is a Sodium Fast Reactor design that will be France's Flagship 4th Generation Reactor.

Its innovative core contains many axial and radial heterogeneities (in order to obtain a negative void coefficient) and interfaces that are challenging for current deterministic codes to simulate correctly. Hence there is the need for new improvements in modeling (3D simulations, parallel processing) like those being elaborated within the APOLLO3® platform.

The APOLLO3-SFR package built with APOLLO3® solvers defines reference calculation schemes associated with a nuclear data library to calculate all neutronic parameters (critical masses, sodium void, Doppler coefficient, βeff, etc…) together with certified biases and uncertainties derived from the VV&UQ process. This VV&UQ process incorporates numerical validation, a-priori uncertainties based on nuclear data covariances as well as experimental validation mainly from MASURCA, a fast mock-up reactor, located at CEA Cadarache.

Innovative numerical scheme based on the use of the sub-group method in a fine energy mesh together with a 2D method of characteristics for calculating the heterogeneous angular fluxes

(real and imaginary with the B1 heterogeneous method) enables a refine core sub-assembly calculation. Clusters are used for sub-critical cells. Cross sections are smeared and condensed on the flux moments for use in the Sn 3D core calculations. Progresses in V&V have shown the high level of accuracy obtained. Further room of progresses are possible with 3D method of characteristics and parallel processing methods for core/subcritical media interfaces.

The use of most recent nuclear data evaluations has shown progresses which will be consolidated and/or improved by the use of integral experiments assimilation techniques especially on capture/fission/inelastic ^{238}U cross section, capture/fission/prompt neutron spectrum ^{239}Pu data and all other heavy nuclei such as ^{240,242}Pu, ^{241}Am.

A future programme called GENESIS will be performed in support to the prototype ASTRID to validate the CFV core specificities such as sodium void reactivity, control rod worth, power map distribution. A part of the GENESIS experimental program contains integral experiment underway at the BFS facility.

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