New Reference APOLLO3 Calculation Scheme for Sodium Cooled Fast Reactors from Sub-Assembly to Full-Core Calculations

P. Archier, J.-M. Palau, J.-F. Vidal, V. Pascal, G. Rimpault, B. Roque, S. Santandrea

NEW REFERENCE APOLLO3® CALCULATION SCHEME FOR SODIUM COOLED FAST REACTORS: FROM SUB-ASSEMBLY TO FULL-CORE CALCULATIONS

P. Archier, J.-M. Palau, J.-F. Vidal,
V. Pascal, G. Rimpault and B. Roque
CEA, DEN, DER, SPRC, Cadarache
Saint-Paul-Lez-Durance, F-13108, France
pascal.archier@cea.fr

S. Santandrea
CEA, DEN, DM2S, SERMA, Saclay
Gif-sur-Yvette, F-91191, France

ABSTRACT

The new reactor analysis platform APOLLO3® is under development at CEA and should replace the current ERANOS code system for Fast Reactor studies. APOLLO3® proposes new solvers and advanced numerical methods to be used for all kinds of reactor concepts. At the same time, CEA is largely involved in the study of the ASTRID project and the CFV core. Thus, new calculation schemes for sodium fast reactor must be defined to predict the main neutronic parameters of this core. This paper presents our new reference calculation route called APOLLO3-SFR and its specificities. Each phase of the scheme is detailed and validated against continuous energy Monte Carlo calculations. Several improvements are foreseen, in particular the development and validation of a partial homogenization method with equivalence and an energy-collapsing procedure involving moments of the angular flux.

Key Words: **Calculation scheme, APOLLO3®, Neutronics, Fast Reactor**

1. INTRODUCTION

A new generation of reactor analysis code, called APOLLO3® [1, 2], is currently developed by the CEA, with the support of EDF and AREVA, and will replace the ERANOS code system [3]. At the same time, the CEA is also involved in the study of the French GEN IV Sodium Fast Reactor ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration) project, which is planned to be built in the 2020's. The CFV concept has been selected to be the ASTRID core and one of its main features consists in a strongly heterogeneous geometry [4] leading to a negative sodium void coefficient (see Figure 1). In this context, a new Sodium Fast Reactor (SFR) reference calculation

scheme is required to precisely predict the main neutronic parameters of the CFV using the recent developments in terms of tools and solvers available in the APOLLO3® code.

In this paper, we will present our new reference calculation route, called APOLLO3-SFR (shortened in AP3-SFR in the following), consisting in a two-phases calculation: sub-assembly calculations followed by core calculations. Each phase is detailed and validated against the reference continuous energy Monte Carlo TRIPOLI-4® [5] code and some improvements in terms of numerical methods are foreseen.

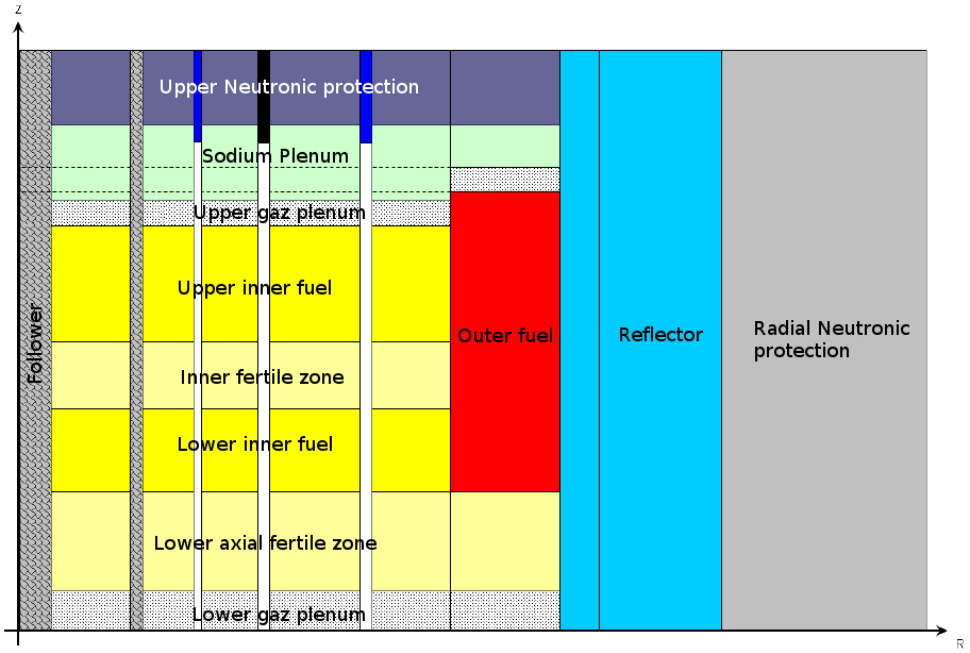

Figure 1. Radial description of the CFV core geometry.

2. SUB-ASSEMBLY CALCULATION SCHEME

2.1. Description of the Scheme

The calculation scheme used at sub-assembly level is presented hereafter: first, the geometries of the fuel, fertile and control rod sub-assemblies are described using the exact geometries (unstructured mesh). Figure 2 presents the different kinds of geometry that are treated by the APOLLO3® code. The symmetry properties of the sub-assemblies (description of only $1/12^{\text{th}}$ of the full geometries) are exploited and allow computational time gains. The fuel sub-assemblies are described alone with reflective conditions. For sub-critical sub-assemblies (fertile, control rod and structural media), we use a geometry defined by a cluster containing at the center the sub-critical sub-assembly surrounding by a ring of fuel sub-assemblies, which are representative of the environment in the core.

The JEFF-3.1.1 nuclear data library is processed with the GALILEE [6] 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. For self-shielding, the probability tables of resonant isotopes, used in the subgroup self-shielding method, are also processed in the same energy mesh structure with the CALENDF code (module of GALILEE).

As said before, the geometry pattern is treated with reflective conditions and no leakage model has been considered for this first scheme, even though a $B1$ homogeneous leakage model is already available in the APOLLO3® code and a B heterogeneous leakage model is under development and validation. This allows a consistent comparison with TRIPOLI-4® for this first version of the scheme.

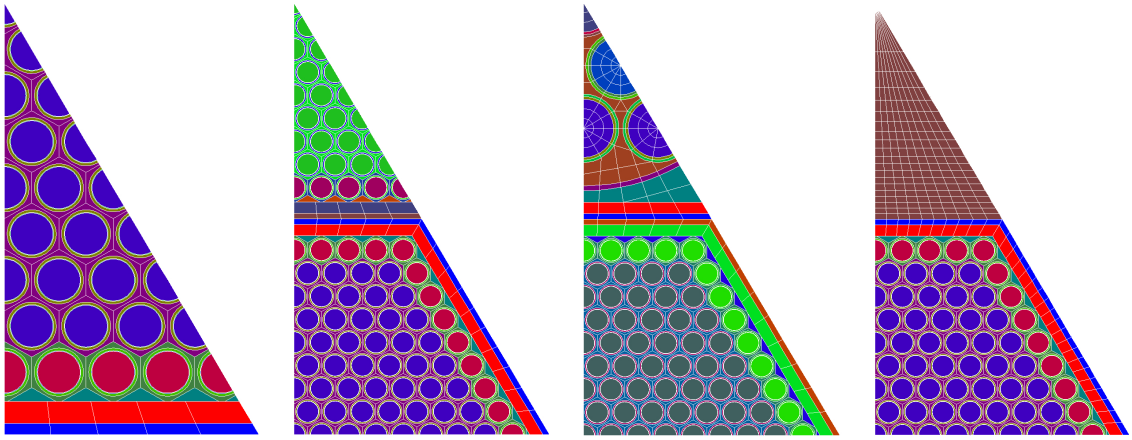

Figure 2. 1/12$^{\text{th}}$ geometries of: a) fuel sub-assembly. b) cluster of sub-assemblies with fertile in the center surrounded by fuel. c) cluster of assemblies with control rod in the center surrounded by fuel. d) cluster of assemblies with homogeneous medium (structural) in the center surrounded by fuel.

The flux calculation is performed with the TDT-MOC [7] solver (Method of Characteristics) with several optimized tracking parameters detailed in Table I to ensure angular and spatial convergences of the flux. We have limited our calculations to P3 Legendre approximation, even though P5 matrices are available (see also Reference [8]).

Table I. TDT-MOC and TDT-CPM tracking parameters

Parameters	Δr	n_ϕ	n_ψ
TDT-MOC	5.0×10^{-2}	24	4
TDT-CPM	1.0×10^{-1}	12	2

This flux solver is coupled with a shelf-shielding procedure, based on the subgroup method and using the probability tables available in the 1968 groups library. A P_{ij} calculation is thus conducted using the TDT-CPM solver (exact P_{ij}) with the same geometry (geometry from the flux calculation and presented in Figure 2). Table I sums up the tracking parameters of TDT-CPM which are less refined than TDT-MOC ones.

Once the convergence on flux is reached, the exact P_{ij} calculation is performed for the self-shielding procedure [8]. Then, the fine and self-shielded cross-sections are collapsed to a larger energy group structure (typically, 33 groups). Also, complete or partial homogenizations of the input geometry are performed. In this scheme, the fuel sub-assembly is completely homogenized. In the case of cluster geometries, the central sub-critical sub-assemblies are fully homogenized but separately from the fuel sub-assemblies environment, without performing an equivalence method afterwards to correct the neutronic balance. Finally, the collapsed and homogenized cross-sections are stored in a Multi-Parametric Output library (MPO), which will be used for core calculations afterwards. Only the cross-sections from the central sub-assembly in cluster geometries will be employed at the core level. The fuel cross-sections come from the fuel sub-assembly calculated in infinite lattice.

2.2. Results and Monte Carlo Validation

Hereafter, we present the main results obtained with our calculation scheme at the sub-assembly level. Those results are compared with the continuous energy Monte Carlo TRIPOLI-4® code [5]. An extended and more detailed validation of this work can be found in Reference [8].

In Table II, we present a synthesis of this validation work in terms of infinite multiplication factors on the fuel sub-assembly geometries (inner and outer fuel). The agreements between the scheme (AP3-SFR) and the reference Monte Carlo results are excellent with a slight over-estimation of the reactivity. Calculation with P1 and P3 Legendre expansions (transfer matrices) have been performed, however the effect in this case is negligible ($\simeq 4$ pcm).

Table II. Infinite multiplication factors (k_∞) for fuel sub-assemblies obtained with AP3-SFR sub-assembly scheme (P1 and P3 anisotropy expansion) and compared to reference Monte Carlo TRIPOLI-4® calculations.

	Inner Fuel Sub-Assembly $\simeq$24 % Pu content	Outer Fuel Sub-Assembly $\simeq$21 % Pu content
k_∞ TRIPOLI-4®(T4)	1.49877 $\pm$ 3 pcm	1.38442 $\pm$ 3 pcm
k_∞ AP3-SFR-P1	1.49900	1.38482
$\Delta\rho$ (AP3-SFR-P1 - T4)	+10 pcm $\pm$ 3 pcm	+21 pcm $\pm$ 3 pcm
k_∞ AP3-SFR-P3	1.49877	1.38491
$\Delta\rho$ (AP3-SFR-P3 - T4)	+14 pcm $\pm$ 3 pcm	+25 pcm $\pm$ 3 pcm

In Table III, multiplication factors calculated for sub-critical sub-assemblies using AP3-SFR are compared with those calculated with TRIPOLI-4®. In those cases once again, the agreement is quite good and we observed a significant improvement using P3 Legendre expansion, especially with the cluster geometry containing fuel and control rod, where the flux gradient can be quite significant.

Table III. Infinite multiplication factors (k_∞) for sub-critical cluster sub-assemblies obtained with AP3-SFR sub-assembly scheme (P1 and P3 anisotropy expansion) and compared to reference Monte Carlo TRIPOLI-4® calculations.

	Cluster subassemblies of…		
	Fuel / Fertile	Fuel / Control Rod	Fuel / Sodium Plenum
Description	Heterogeneous	Heterogeneous	Het. / Hom.
TRIPOLI-4®(T4)	1.30318 ± 3 pcm	1.06453 ± 2 pcm	1.45040 ± 3 pcm
k_∞ AP3-SFR-P1	1.30289	1.06255	1.45035
$\Delta\rho$ (AP3-SFR-P1 - T4)	-17 pcm ± 3 pcm	-175 pcm ± 2 pcm	-2 pcm ± 3 pcm
k_∞ AP3-SFR-P3	1.30355	1.06395	1.45061
$\Delta\rho$ (AP3-SFR-P3 - T4)	22 pcm ± 3 pcm	-51 pcm ± 2 pcm	10 pcm ± 3 pcm

3. CORE CALCULATION SCHEME

3.1. Description of the Scheme

The self-shielded cross-sections, necessary to perform a full core calculation, have been prepared at the sub-assembly level (see Section 2). They have been collapsed in energy to a broad group structure (in this paper, 33 groups) and homogenized for each sub-assembly. We then used the transport Sn solver MINARET [9] for the core calculation. The characteristics of this solver can be summarized as follows: discrete ordinates method (angular discretization), discontinuous Galerkin finite elements applied on unstructured spatial meshes with triangular extruded cells.

MINARET also contains several features to speed up the resolution of the transport equation: MPI parallel computation (parallelism on angular directions), DSA method and Chebyshev acceleration. For this study, all these parameters have been optimized to reach angular and spatial convergence: S8 level-symmetric quadrature (120 directions), first order polynomial function of the DGFEM method to describe the flux on the spatial level, 5 cm for the axial discretization and 18 triangles by hexagon (radial discretization) which leads to about 920,000 cells for the calculation mesh (in the case of the nominal core configuration).

Several configurations of the CFV core have been studied here: the nominal configuration with control rods withdrawn, a voided situation (same position for the control rods) and a configuration where the control rods are inserted.

At the sub-assembly level, the fuel and blanket sub-assemblies have been treated with the exact heterogeneous geometries (*cf.* previous section). In order to investigate the control rods worth, two geometries for the control rod sub-assembly have been considered: one homogeneous and one hetero-

geneous[1]. To validate the core scheme, we used TRIPOLI-4® on the same core geometries, with the fuel, blanket (and possibly the control rods) explicitly described.

3.2. Results and Monte Carlo Validation

We present hereafter the validation and associated results compared to TRIPOLI-4® Monte Carlo calculation. The first geometry model (named `Geo1`) contains the fuel (inner and outer), the blanket detailed explicitly and homogenized control rods. The second geometry, `Geo2`, is the same as `Geo1` but with the control rods also described explicitly.

3.2.1. Results on `Geo1`

Table IV shows results obtained from our AP3-SFR core scheme using several Legendre order expansion (P1 and P3) compared to TRIPOLI-4® reference calculations. We can see that the agreement on multiplication factors worsen systematically using P3 anisotropy instead of P1 scattering matrices, especially in the voided configuration. However, the $\Delta\rho_{\mathrm{Na}}$ and $\Delta\rho_{\mathrm{CR}}$ seem to be less sensitive to the anisotropy order.

Table IV. Multiplication factors (k_{eff}) and reactivity effect ($\Delta\rho$) for nominal, voided and inserted control rods (CR) configurations, calculated on `Geo1` using AP3-SFR core scheme (P1 and P3 anisotropy expansion) and compared to reference Monte Carlo TRIPOLI-4® calculations.

Configuration	Nominal	Voided		Inserted Control Rods	
Parameter	k_{eff}	k_{eff}	$\Delta\rho_{\mathrm{Na}}$ (pcm)	k_{eff}	$\Delta\rho_{\mathrm{CR}}$ (pcm)
TRIPOLI-4	1.05408 $\pm$ 2 pcm	1.04533 $\pm$ 2 pcm	-794 $\pm$ 3	1.02836 $\pm$ 2 pcm	-2372 $\pm$ 3
AP3-SFR-P1	1.05575	1.04899	-610	1.03075	-2297
$\Delta\rho$ (AP3-SFR-P1 - T4)	+150 $\pm$ 2	+334 $\pm$ 2	+184 $\pm$ 3	+225 $\pm$ 2	+75 $\pm$ 3
AP3-SFR-P3	1.05693	1.05054	-575	1.03199	-2287
$\Delta\rho$ (AP3-SFR-P3 - T4)	+256 $\pm$ 2	+474 $\pm$ 2	+219 $\pm$ 3	+342 $\pm$ 2	+85 $\pm$ 3

This result, even though the cross-sections are more precise with P3 Legendre order, may be due to the energy-collapsing method performed at the sub-assembly step. The latter uses the scalar flux to collapse the scattering matrices instead of the angular flux and does not take into account the flux gradient (and the leakage), in particular in the case of cluster geometries. In the near future, we plan to validate a newly developed collapsing method in APOLLO3® using the moments of the angular flux [10]. Moreover, the 2D cluster geometries are not fully representative of the core environment. Thus, 3D TDT-MOC assembly calculations have been performed to validate this assumption and work in progress are detailed in Reference [11]. Finally, the partial homogenizations (for cluster geometries) at the end of the sub-assembly step have been performed without using any equivalence method and may be necessary to correct the cross-sections to preserve the neutronic balance.

[1] It means that the control rod sub-assembly is heterogeneously described at the sub-assembly level, as depicted in Figure 2, than homogenized for the core calculation.

3.2.2. Results on Geo2

Calculation results on Geo2 are compared in Table V between the AP3-SFR core scheme using only P3 anisotropy order and TRIPOLI-4®. The agreement on multiplication factors is globally improved with respect to results in Table IV, especially for the nominal and control rod cases. The $\Delta\rho_{\mathrm{CR}}$ with AP3-SFR is slightly overestimated but the result seems sufficient, it means that the heterogeneous calculation of the control rods at the sub-assembly level could prevent us to perform a reactivity equivalence method. Concerning the $\Delta\rho_{\mathrm{Na}}$, we can see that the biais is more significant with this geometry, probably for the same reasons raised previously for Geo1.

Table V. Multiplication factors (k_{eff}) and reactivity effect ($\Delta\rho$) for nominal, voided and inserted control rods (CR) configurations, calculated on Geo2 using AP3-SFR core scheme with P3 anisotropy expansion and compared to reference Monte Carlo TRIPOLI-4® calculations.

Configuration	Nominal	Voided		Low Position CR	
Parameter	k_{eff}	k_{eff}	$\Delta\rho_{\mathrm{Na}}$ (pcm)	k_{eff}	$\Delta\rho_{\mathrm{CR}}$ (pcm)
TRIPOLI-4	1.05689 $\pm$ 2 pcm	1.04693 $\pm$ 2 pcm	-900 $\pm$ 3	1.03478 $\pm$ 2 pcm	-2021 $\pm$ 3
AP3-SFR-P3	1.05885	1.05193	-621	1.03609	-2075
$\Delta\rho$ (AP3-SFR-P3 - T4)	+175 $\pm$ 2	+454 $\pm$ 2	+279 $\pm$ 3	+122 $\pm$ 2	-54 $\pm$ 3

4. CONCLUSION AND PERSPECTIVES

In this paper, our new reference sub-assembly to core calculation scheme for Sodium Fast Reactor, called APOLLO3-SFR, has been presented. Each one of those two steps has been detailed and several elements of validation against continuous energy Monte Carlo have been shown. For the sub-assembly step, the results obtained with AP3-SFR scheme are very close (few dozens of pcm) to the TRIPOLI-4® ones. At the core level, the prediction of the neutronic parameters is less satisfactory and the main reasons may be due to the homogenization and energy-collapsing methods used at the end of the sub-assembly level.

In terms of perspectives, several improvements are foreseen ; in particular a new cross-sections collapsing method involving the moments of the angular flux is already implemented in APOLLO3® and currently in validation. This method should guarantee a better neutronic balance. Also, a transport/transport equivalence method should be performed in order to preserve the neutronic balance when partial homogenizations (for cluster geometries) are carried out. Finally, we plan to have a more detailed geometry at the core level (see for instance Figure 3 where the control rods sub-assembly are explicitly described) to take into account the numerous spatial heterogeneities (radial and axial) of the CFV and their effects on the neutronic parameters.

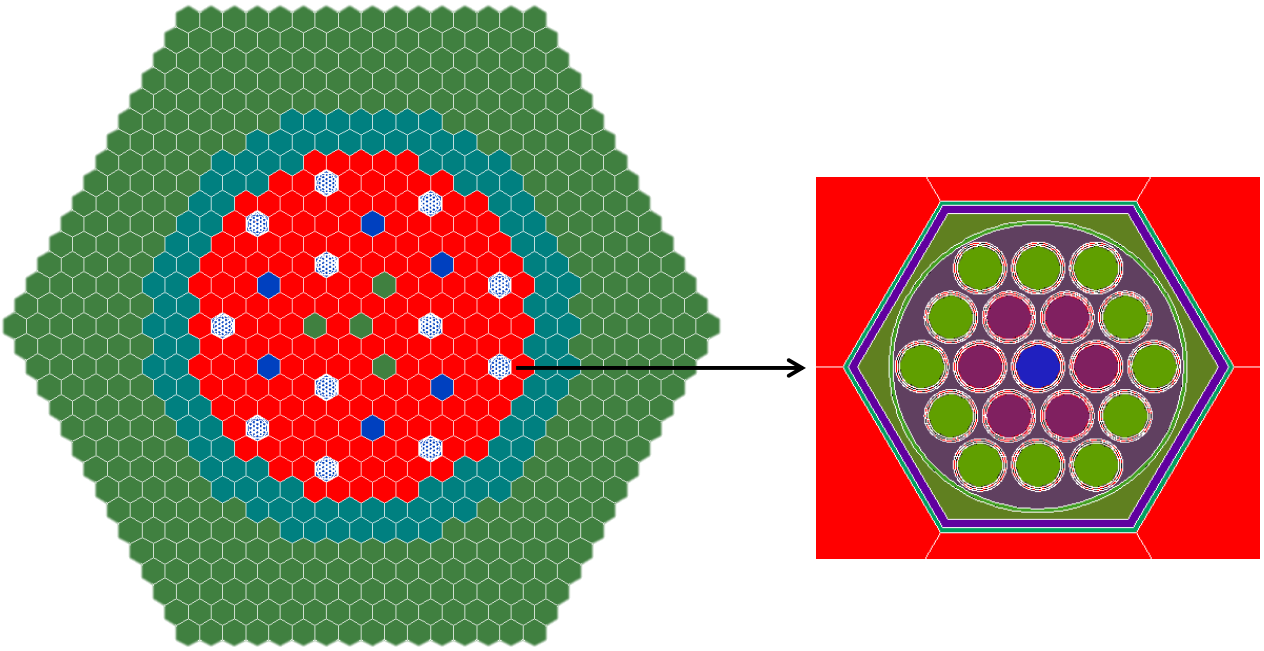

Figure 3. Example of a radial description of a CFV core geometry, where the control-rods sub-assemblies are explicitly described.

ACKNOWLEDGMENTS

The authors would like to thank the APOLLO3® development team for their efforts in developing the code. APOLLO3® is a registered trademark of CEA. We gratefully acknowledge AREVA and EDF for their long term partnership and their support.

REFERENCES

[1] H. Golfier *et al.* "APOLLO3: a common project of CEA, AREVA and EDF for the development of a new deterministic multi-purpose code for core physics analysis." In: *International Conference on Mathematics, Computational Methods and Reactor Physics (M&C 2009)*. American Nuclear Society (ANS). Saratoga Springs, New York, USA, May 3 - 7 (2009).

[2] D. Schneider *et al.* "APOLLO3®: CEA/DEN Deterministic Multi-Purpose Code for Reactor Physics Analysis." In: *This PHYSOR 2016 Conference*. Americal Nuclear Society. Sun Valley, Idaho, USA, May 1 - 5 (2016).

[3] J.-M. Ruggieri *et al.* "ERANOS 2.1: International Code System for GEN IV Fast Reactor Analysis." In: *ICAPP 2006 - International Congress on Advances in NPPs*. American Nuclear Society. Reno, Nevada, USA, June 4 - 8 (2006).

[4] C. Venard *et al.* "The ASTRID Core at the Midtime of the Conceptual Design Phase (AVP2)." In: *ICAPP 2015 - International Congress on Advances in NPPs - Nuclear Innovations for a Low-carbon Future*. French Nuclear Energy Society (SFEN). Nice, France, May 3 - 6 (2015).

[5] E. Brun *et al.* "TRIPOLI-4®, CEA, EDF and AREVA reference Monte Carlo code." *Annals of Nuclear Energy*, **82**: pp. 151–160. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013, SNA + MC 2013. Pluri- and Trans-disciplinarity, Towards New Modeling and Numerical Simulation Paradigms (2015).

[6] M. Coste-Delclaux. "GALILEE: A nuclear data processing system for transport, depletion and shielding codes." In: *PHYSOR 2008 - Nuclear Power: A Sustainable Resource*. Americal Nuclear Society. Interlaken, Switzerland, September 14 - 19 (2008).

[7] F. Févotte, S. Santandrea, and R. Sanchez. "Tracking on periodic lattices for the method of characteristics." In: *PHYSOR 2008 - Nuclear Power: A Sustainable Resource*. Americal Nuclear Society. Interlaken, Switzerland, September 14 - 19 (2008).

[8] J.-M. Palau *et al.* "Recent progress in the V&V process of the new CEA APOLLO3 code: advanced multi-spectrum assembly calculations." In: *This PHYSOR 2016 Conference*. Americal Nuclear Society. Sun Valley, Idaho, USA, May 1 - 5 (2016).

[9] J.-Y. Moller and J.-J. Lautard. "MINARET, a Deterministic Neutron Transport Solver for Nuclear Core Calculations." In: *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011)*. Latin American Section (LAS) / American Nuclear Society (ANS). Rio de Janeiro, Brazil, May 8 - 12 (2011).

[10] J.-F. Vidal *et al.* "An Improved Energy-Collapsing Method for Core-Reflector Modelization in SFR Core Calculations Using the Paris Platform." In: *PHYSOR 2012 - Advances in Reactor Physics - Linking Research, Industry, and Education*. American Nuclear Society. Knoxville, Tennessee, USA, April 15 - 20 (2012).

[11] P. Archier *et al.* "Validation of the Newly Implemented 3D TDT-MOC Solver of APOLLO3® Code on a Whole 3D SFR Heterogeneous Assembly." In: *This PHYSOR 2016 Conference*. Americal Nuclear Society. Sun Valley, Idaho, USA, May 1 - 5 (2016).