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## **APOLLO3<sup>®</sup>: CEA/DEN deterministic multi-purpose code for reactor physics analysis**

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### **ABSTRACT**

APOLLO3<sup>®</sup> is a common project of CEA, AREVA and EDF for the development of a new generation code system for core physics analysis providing improved accuracy, flexible software architecture and high computation performances and taking into account both R&D and industrial application requirements. This paper presents the most important developments implemented in the deterministic APOLLO3<sup>®</sup> code, and their validation.

APOLLO3<sup>®</sup> provides new capabilities from spectral aspect up to core calculations and a large panel of solvers adapted for different applications.

This paper discusses the general architecture of the software platform, the data libraries, models of cross section self-shielding and solvers implemented in APOLLO3<sup>®</sup>. The last part of this paper describes the verification and the validation of that platform and examples of use cases: PWR (Pressurized Water Reactor) and SFR (Sodium Fast Reactor) applications.

*Key Words:* **deterministic transport code, APOLLO3<sup>®</sup>, V&V, SFR, PWR**

## 1. INTRODUCTION

This paper presents the most important developments implemented in APOLLO3<sup>®</sup>, the new multi-purpose deterministic nuclear code under development in the frame of the neutronics simulation project of the nuclear division energy (DEN) of the CEA and with financial support from AREVA and EDF [1]. It displays a common and unique organization for the “spectral” and “core” simulations of nuclear reactors and allows efficient realization of classical or advanced schemes.

Several challenges have induced CEA development teams to develop APOLLO3<sup>®</sup>, especially those related to the modeling of new nuclear reactor types displaying very heterogeneous cores, innovating fuels and a wide variety of geometries such as the sodium fast reactor ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration) or the experimental reactor JHR (Jules Horowitz Reactor). Indeed, the requirements formulated by the 4th Generation reactor designers are highly stimulating and structuring since they assign new objectives to R&D. Moreover, computer architecture and processor power are significantly progressing. These progressions, combined with an optimum structuration of the code architecture, the development of new algorithms and numerical methods to significantly reduce the computational times and the used required memory sizes could already put in perspective the key goals of neutronics code development, being able to perform a full reactor’s core in a single step.

In this paper, we focus on the presentation of the main features of the codes. Section 2 is related to the general architecture of the software. The external data libraries and cross section self-shielding methods (fine structure formalism, sub-groups method, resonant mixture and resonant up-scattering) are discussed in section 3. Section 4 deals with the main feature of flux solvers while section 5 gives a brief summary of V&V achievement. Section 6 illustrates the capability of APOLLO3<sup>®</sup> for the calculation schemes of PWR and SFR reactors. We conclude with some comments and perspectives in section 7.

## 2. ARCHITECTURE

The code is mainly based on object oriented design and C++ programming language. The software architecture design chosen in APOLLO3<sup>®</sup> is a layered architecture consisting of several functional and modular components. The different layers can be represented by the following ones:

- The TEST layer: contains all the tests
- The CONTROLLER layer: control of the application, the chains top-level and the majority of the API
- The SOLVER layer: contains all available solvers
- The DATA layer: contains internal data
- The TOOLS layer: contains a set of tools usable by all other layers

Each of these layers can contain one or several components and the components of top layers can call the components of the same or the lower layers.

Three standalone ways of uses are possible:

- A C++ programming language;
- An interpreted language Python with the same level as the C++ way;
- A language keyword/value text.

A supplementary possibility of use is offered by the creation of an APOLLO3<sup>®</sup> application which can be integrated in the SALOME platform [26] to perform coupling calculations with others codes for multi-physics simulation [28].

### 3. NUCLEAR DATA AND SELF SHIELDING

Uploading isotopic physical data is the starting point for the APOLLO3<sup>®</sup> lattice calculation. At the present time, four external-library files are provided for the storage of the nucleus cross-sections, for the self-shielding data, for the depletion data and for the kinetic parameters. Those libraries are provided by the CEA GALILEE [5] platform which allows producing coherent data from any evaluated nuclear data file in ENDF format for the different CEA codes.

The External-Library Files for Neutron microscopic Cross Sections (ELFN-XS) is based on a hierarchical structure for efficiently handling of temperature-dependent cross sections on fine multigroup structure (from hundreds to thousands of energy groups.) The number of reactions as well as the temperature mesh and the inventory of the released energies are all isotope-dependent.

The principal aim of the resonance self-shielding calculations of APOLLO3<sup>®</sup> is being capable of calculating both, the thermal and the fast reactors.

The Fine Structure (FS) method based on equivalence theory is able to perform the resonance self-shielding for the thermal reactor calculations. The method designed for the APOLLO2 code [2] [4], has been improved for the APOLLO3<sup>®</sup> code. The APOLLO2 method has been adapted to take into account resonant up-scattering treatment in APOLLO3<sup>®</sup> [6]. For that, improvements in resonance interference treatment have been performed [3]. For the fast reactor, the first self-shielding method implemented in APOLLO3<sup>®</sup> is the subgroup method (the same formalism as implemented in the ECCO code [7] [14] [24]) where the self-shielding is calculated simultaneously with the most recent multigroup flux obtained in the  $k_{\text{eff}}$ -iteration.

### 4. SOLVERS

The APOLLO3<sup>®</sup> multigroup transport code was written incorporating and extending the capabilities of the original codes APOLLO2 [2] [8], CRONOS2 [8] and ERANOS2 [24]. The code is written mainly in C++ and FORTRAN 90.

For lattice calculation, standard flux calculation methods such as collision probability model (multicell approximation with interface current method or direct 2D exact geometry), short and long characteristics method have been implemented. The short (IDT – [12][15]) and long (TDT - [9][10][11][13][14]) characteristic methods are currently extended in 3D. Speed up is achieved using acceleration techniques or by parallelizing the algorithms with OpenMP directives. All solvers

take into account leakage models such as the B1 homogeneous. A B1 heterogeneous leakage model has been recently implemented for the TDT solver. A reconstruction flux method is also available as a standard module. Output cross sections can be obtained using homogenization techniques such as flux-volume method, SPH or Selengut but also a homogenization using the moment of the angular flux. Techniques such as SPH and Selengut are driven by the solver used at the core calculation level, the lattice level providing only reference reaction rates.

For core calculation, several solvers can be used according the technical specificities of the problem to be solved. The flux core calculation can be computed using the solver MINOS [17] which treats the SPN or diffusion approximation of the 3D transport equation for steady-state, kinetics or perturbation calculations for cartesian and hexagonal 3D geometries. This solver is based on the mixed dual finite element approximation (Raviart-Thomas-Nedelec elements). In order to speed up calculations using a great number of meshes, an iterative domain decomposition method (IDD) [18][19] has been implemented.

The flux distribution can also be computed, especially for sodium fast reactor having 3D hexagonal geometries with the nodal Pn solver PASTIS. A finite element solver called MINARET [16][20][21][22] allows performing 2D/3D transport SPN or SN calculation on unstructured cylindrical geometries. The spatial discretization uses the discontinuous Galerkin finite elements approximation. Taking into account the independency of each directional sweeping, a parallel algorithm has been implemented using MPI message passing library. In this case, the SN directions are distributed on the different available processors. The transport source calculation is accelerated via a standard DSA algorithm using the same spatial discretization and the same discontinuous finite element approximation, SPN and diffusion calculations are made possible by using DSA matrices and by skipping the transport sweep.

A generic perturbation module using all these core solvers can also be used to perform perturbation analysis.

A generic kinetics module is also implemented for MINOS and MINARET solvers [29].

For isotopic depletion calculation, all lattice and core solvers are coupled with the MENDEL-solver library [23] which solves the multi-group Bateman equations.

## 5. V&V

The V&V process is based on a two-steps approach and “Physical Identification Ranking Tables” which cover a large range of LWR, SFR and MTR (Material Testing Reactor) applications. The first, Verification step, aims at checking all programming functions and resolution models (a dedicated test machine called CAT2 is used to check non regression between the incremental versions of the code). The second, Validation step, aims at ensuring numerical convergence of these deterministic methods (towards Monte-Carlo or experimental references) and assess (i.e. quantify) the global performance of the code for calculating 1D to 3D cell/assembly/core configuration of a large panel of reactor applications (what we call Master Classes: LWR/SFR/MTR).

The most recent V&V results highlighted the capability of the code to predict the main physical

parameters with at least the same accuracy of the previous generation in the case of representative cell/assembly and core LWR/FBR geometries [33]. In the latter case (FBR) some relevant geometry issue (2D/3D strong heterogeneities) have been overcoming with the use of unstructured flux solver (such as TDT-MOC and Minaret solvers used at assembly and core calculation step respectively).

Previously a benchmarking campaign showed the versatility of transport flux solvers to deal with various 1D to 3D core geometries [31].

### First V&V results (synthesis)

The first V&V work [31] focused on the main transport flux solvers of the code (IDT, TDT, Minos, Minaret and Pastis) through 1D to 3D international benchmarks (ZPR-1D, Stepanek, C5G7, Takeda). Precise criteria have been defined to assess the quality of each solver by comparison with TRIPOLI4<sup>®</sup> multigroup Monte-Carlo calculations that have been performed for each configuration. It was shown that pure transport flux solvers (IDT, TDT-MOC, Minaret and Pastis) based on  $S_n$ ,  $P_n$  and characteristics methods meet the  $k_{\text{eff}}$  target precision criteria (100 pcm) whereas  $SP_n$  solvers (Minos/Minaret) give satisfactory results within reasonable computation time (lower than 400 pcm dividing by 3 the computation time compared with pure  $S_n$  transport solvers). The complementary of the APOLLO3<sup>®</sup> flux solvers set is globally highlighted (each benchmark can be treated successfully by at least one flux solver).

The next V&V exercise (based on the v1.2 version under-development) was devoted to cell/assembly calculations and will be presented in this conference [33].

## 6. APPLICATIONS

### 6.1. PWR applications

#### 6.1.1 Simulation of the first cycle of Saint Laurent B1

The aim of this exercise was to illustrate the possibilities of the APOLLO3<sup>®</sup> code to calculate a PWR reactor cycle on the example of the first cycle of one of EDF's reactor, St Laurent unit B1, using a conventional two-step scheme.

(1) Lattice calculations: Pin by pin assemblies' transport calculations in different operating conditions to compute and store the homogenized cross sections in the form of libraries called Multi-Parameter Output (MPO). Calculations were performed by using the MOC transport method with a 281 energy groups library and a depletion chain containing separated filiations of 229 isotopes.

(2) Core calculations: The calculation was performed with a two groups, 3D  $SP_N$  Minos solve. The spatial mesh was composed of 4x4 radial subdivisions in each assembly, 32 axial plans in its active part.

#### Results

The core depletion calculation with thermo-hydraulic feedbacks was performed with the critical boron search and the control rod movement features. The outputs of this simulation were the critical boron concentration and the power map during the cycle, with a simplified control rod operating, control rods efficiency and isothermal coefficient.

### 6.1.2 Advanced modeling reflector

The "best-estimate" calculation of a big core (241 assemblies) integrating advanced modeling of the reflector was performed with APOLLO3<sup>®</sup> code. The objective was to produce a 2D and 3D model of the core with a fine modeling of the geometry of the reflector. The exercise was performed using a core description with a cell-by-cell geometry on the one hand and with a geometry describing the reflector on the other hand. The post-processing of the results allowed editions of flux and power maps on different geometries levels.

To limit the computational time, the decomposition domain multi-Solver (MINOS and MINARET) and works to parallelize the DSA calculations by domain decomposition axially and radially are being developed.

### 6.1.3 Multiscale and multi-solver pin power reconstruction approach in a reactor core calculation

This study [29] was part of a work carried out in order to analyze PWR Nuclear reactor behavior in cases of standard and accidental (REA) situations through a multi-physics "Best Estimate" modeling. This work uses the SALOME [26] platform which allows the coupling of APOLLO3<sup>®</sup> with the thermos-hydraulic code FLICA4 [8] [25], dedicated to best-estimate modeling of Pressurized Water Reactor (PWR) in normal and accidental situations. One of the goals of this work was to get access to the local parameters at the fuel pin and sub channel scale. The other one was to properly and efficiently couple the different physics. The transient calculation was based on a coupled calculation between MINOS-SP<sub>N</sub> and MINARET-S<sub>N</sub>.

## 6.2. SFR applications

A first 3D coupled neutronics – fuel mechanics with APOLLO3<sup>®</sup> and GERMINAL code was performed for rod withdrawal transient in a heterogeneous SFR [27]. These calculation schemes open the way for best estimate rod withdrawal transient analysis. This simulation was based on APOLLO3<sup>®</sup> best-estimate deterministic neutron transport code and GERMINAL best-estimate fuel physics code. In particular, a 3D time dependent calculation was used for coupled simulations thanks to new software, architecture and dedicated coupling platforms with parallel simulation capabilities.

First implementation steps for coupled 3D time dependent neutronics and pin-scale transient fuel behavior are presented in [27]. Since then, others applications, particularly in the context of ASTRID studies have been carried out with APOLLO3<sup>®</sup> code.

## 7. CONCLUSIONS

Even if the APOLLO3<sup>®</sup> code is still under development, its uses are gaining speed as illustrated by the papers submitted to this conference [32][33][34][35][36][37][38][39][40][41][42][43]. The current version allows to cover the main conception needs for PWR and ASTRID reactor. It though offers more innovative capabilities than the code of the current generation (fully transport calcula-

tion on exact geometry with large group number). Efforts are ongoing to optimize time calculation and the memory print, especially to face new hardware architecture. A roadmap sets short-term objectives, one of these being the capability to calculate configuration far from the fundamental mode by flux and current exchange between lattice and core level computations. A more long-term goal is to be able to perform a calculation core transport 3D bypassing the classical scheme in two steps.

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