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APOLLO3: a common project of CEA, AREVA and EDF for the development of a new deterministic multi-purpose code for core physics analysis

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ABSTRACT

During the last decade, the interest in the nuclear industry for improved nuclear code systems has been growing. Based on an assessment of different reactor concepts (PWR, BWR, GFR, SFR, SCWR…) and of operating margins to cover uncertainties, the development of a new deterministic multi-purpose code APOLLO3 has been launched including lattice, core and lattice-core applications. In addition, the constant increase in high performance computing resources and in the ability to perform calculations on parallel computers gives new guidelines and opportunities for the development of the future code and for the extension of the methods to solve large-scale deterministic problems. APOLLO3 is a common project of CEA, AREVA and EDF for the development of 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.

Key Words: deterministic multi-purpose code, physics analysis, APOLLO, CRONOS, ERANOS, reactor concept (PWR, BWR, GFR, SFR, SCWR…), R&D, project and industrial schemes

1. INTRODUCTION

During the last decade, there has been a growing interest in the nuclear industry for improved nuclear code systems. Based on an assessment of the design of different reactor concept (PWR, BWR, GFR, SFR, SCWR…) and of operating margins to cover uncertainties, there has been a growing interest for the development of a new deterministic multi-purpose code including Lattice, Core and Lattice-Core calculations.

In addition, the evolution of the computer mainframe industry has proceeded along different lines with respect to hardware development. Thus, it is possible to benefit from the constant

increase in high performance computing resources and particularly in the ability to perform calculations on parallel computers. It will give new guidelines for the development of future codes and for the extension of the methods to solve large-scale deterministic problems. Within the neutronic modeling framework, important evolutions are required with regard to energy mesh structure, extension of numerical methods, new applications... It appears that the boundary concition (external and internal) should become an essential aspect for the implementation of multi-solver methods and parallelized calculations. A complete and coherent nuclear system must be considered from nuclear data treatment tools to calculation codes (deterministic and Monte-Carlo codes). According to the codes and the applications, the uncertainties data treatment plays an important role.

Up to now, CEA, with EDF and AREVA support, is renewing its main application codes (deterministic codes "APOLLO2, CRONOS2, and ERANOS2" [1, 2, 3, 4, 5, 6], Monte Carlo code TRIPOLI-4 [7], depletion and fuel cycle Code_DARWIN3 [8], its nuclear data processing system GALILEE in order to have a complete and advanced nuclear modeling system (see Figure 1) and CONRAD, a nuclear reaction analysis tool in order to create evaluations [39].

In order to reach a new stage in the modeling of the nuclear systems a new generation of codes will be developed on an approach where core/lattice, deterministic/Monte-Carlo, reference/industrial calculation routes are compatible.

APOLLO3 is a common project of CEA, AREVA and EDF for the development of new generation system for core physics analysis. Therefore, requirements both for R&D and industrial applications were taken into account for the design of the new system architecture. The new system APOLLO3 is the continuation of the “APOLLO2, CRONOS2, and ERANOS2” code family [1, 2, 3, 4, 5, 6]. The experience on APOLLO2, CRONOS2, ERANOS2 codes and their applications provides an initial and complete set of calculation routes for the neutronic evaluation; this experience draws the ways of improving the models (flux solvers and self-shielding methods with new acceleration or effective parallelization methods…).

In order to meet these objectives, the main APOLLO3 requirements are the following:

- Flexibility: from best-estimate calculations to industrial design;
- Coupling with codes from other disciplines (thermal-mechanics, thermal-hydraulics) with SALOME platform [29];
- Easy coupling with Monte-Carlo codes: in particular with TRIPOLI [7] through a dedicated shared data interface;
- Extended application domain: criticality, shielding of all types of reactors (PWR, BWR, GFR, SFR, SCWR…);
- Uncertainties assessment with perturbation methods and non-intrusive methods (i.e. URANIE [34]);
- Ability to perform calculations on parallel computers;
- User friendly: user interface, databases…
- Portability

This paper comprises four parts. In the first one, the objectives and the innovations are listed. The second one is devoted to a brief description of the main solvers implemented within the APOLLO3 platform, the general architecture of the software platform and the internal data model. To illustrate the potential of the present APOLLO3 code which is under development, some examples of applications are illustrated in the third part. The last section deals with the Verification&Validation process for the future available release of APOLLO3 code.

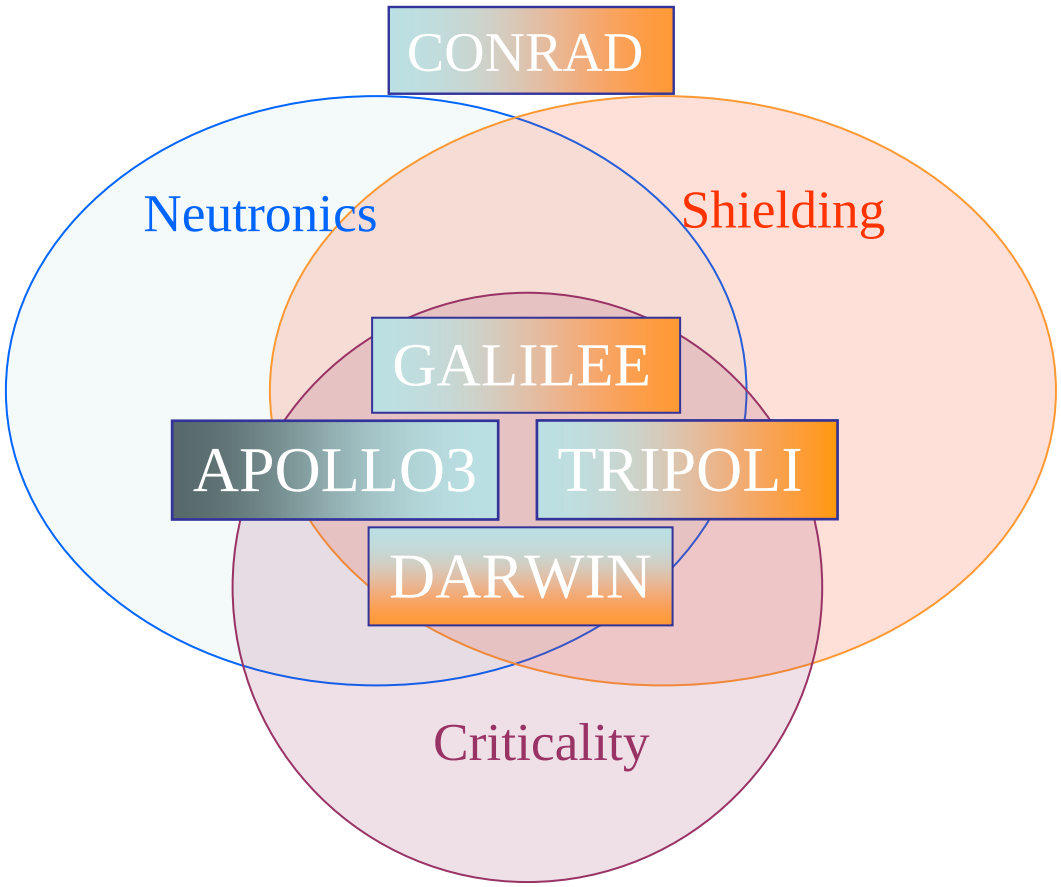


Figure 1. CEA global development program dedicated to fine neutronic modeling of nuclear systems

2. PROGRAM AND MAIN MILESTONES

The main objectives which led the current development of APOLLO3 are the following:

- To preserve continuity with actual system codes (APOLLO2, CRONOS2 and ERANOS2 codes) improving rationalization;

- To implement new transport 3D solvers and new functionalities (i.e. perturbations, kinetic, equivalence theory) in order to achieve both industrial and reference computational routes.

The main milestones are the following, summarized in Figure 2.

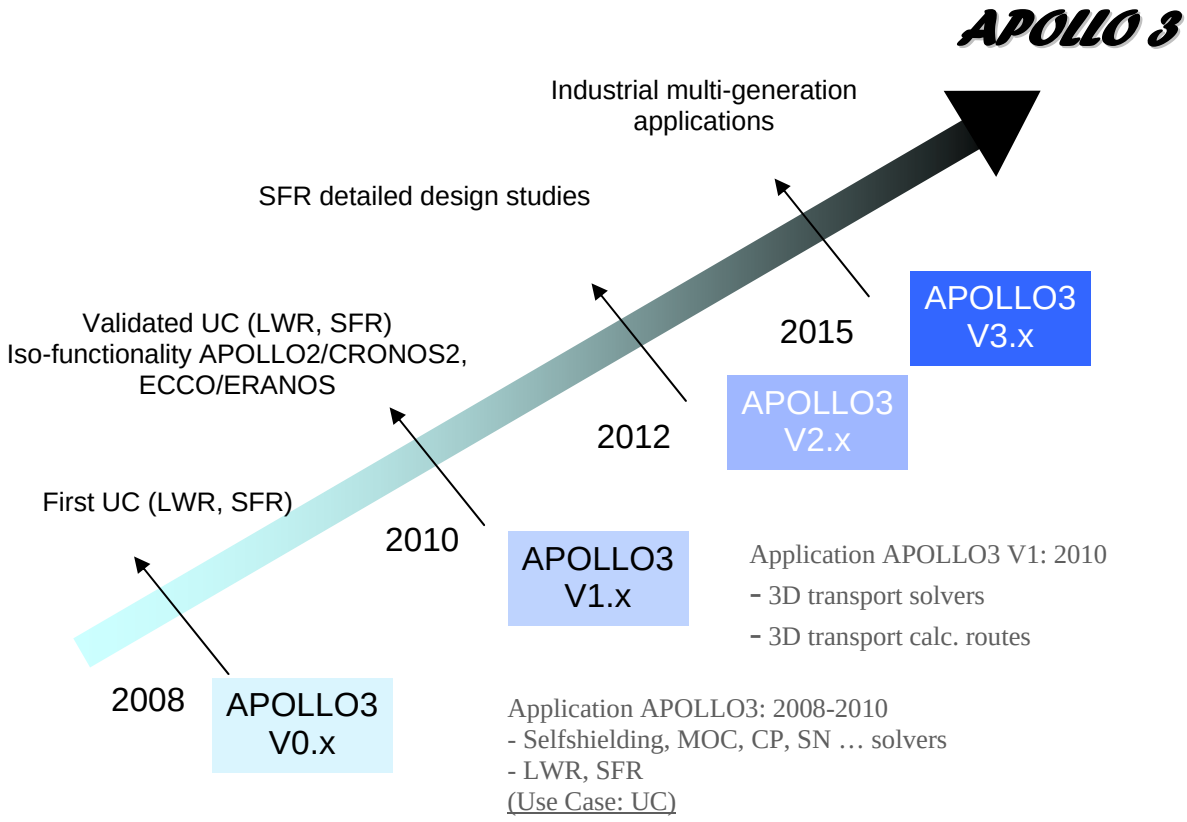


Figure 2. Main milestones

3. ORIENTATIONS AND NUMERICAL METHODS

The APOLLO3 code scope will cover all reactor types including LWR, FBR analysis. Many development axes are currently being pursued, like advanced lattice and core solvers, parallel computation and functionalities for various types of reactors.

From the industrial point of view, the general trend in LWR core and fuel design towards greater heterogeneity, higher enrichment values, burn-up, burnable poison-loading, MOX loading, low leakage configurations, etc. will require higher accuracy in physics modeling. Moreover, the evolution of safety study methodologies towards full 3D neutronics – thermal-hydraulics – thermal-mechanics models to reduce the penalizations and improve operation margins will bring the need for suitable robust coupled code systems. The capability of modeling new designs such

as the Generation IV concepts (FR, HTR) as well as of performing R&D studies and the validation process (requiring fine energy and spatial mesh…) will be essential to prepare for future nuclear power production scenarios.

Different approaches to uncertainty and sensitivity analysis have been established to evaluate the reliability of code calculation, taking into account the possible sources of error; i.e. propagation of code-input uncertainties and of code-output errors. In order to identify and to assess the observed deviations between the measurement and the code calculations, uncertainty and sensitivity calculations depend on many aspects. On the other hand, the most meaningful evolutions in neutronics field associated to computational means led to some guidelines towards new methodological and design approach (i.e. 3D MOC transport solver) and in the way to justify the design (uncertainties, instrumentation). Finer modeling requires both more precise nuclear data and more complex numeric solutions with respect to computational time, memory requirement... The main functionalities are derived from APOLLO2, CRONOS2 and ERANOS codes. The main objectives are to renew the current CEA codes and to overcome the actual limitations to extend fine and unstructured resolution methods (MOC and FEM) to whole 3D core simulations. One notes limitations inherent to methodology (complicated modeling scale as zoom and local refinement; limitation to 2D geometry) and inherent to software architecture (a two step calculations with a lattice followed by core calculations; a real separation of lattice and core codes; no sufficient links between solvers as Monte Carlo, Pij, Sn, SPn, Pn solvers; data required for coupling with other disciplines not included in internal data structure of current neutronic codes).

The main guidelines for the development of the different solvers are the following:

- To fulfill the needs for PWR, BWR, GFR and FBR (2D/3D, with detailed modeling of specific features like cladding, absorber rods, truncated fuel rods, reflector…);
- To elaborate cross section libraries in a few hundred and thousand of energy groups with effective cross sections using Livolant-Jeanpierre model, sub-group method, using a fine energy structure for resonance overlapping energy range;
- To enhance control rod, reflector modeling ;
- To generalize multi-assembly and core depletion calculations allowing for full-core transport;
- To improve and implement solvers in order to provide the computational routes from fast industrial calculations with maximum performance to very accurate reference calculations with lattice calculation precision;
- To factorize and share functionalities and solvers like homogenization, energy collapsing, perturbations, kinetics, equivalence…;
- To improve multi-purpose usage, versatility and generic processes, as for instance unified tracking for the method of characteristics and the collision probabilities solvers;
- To improve the prediction of complex phenomena that occur in various applications and to reduce uncertainties within coupled neutronic - thermal-hydraulic 3D kinetic applications, fuel modeling;
- To have the capability to calculate cross sections by taking into account the core environment and on-the-fly calculational process.

3.1. Physical models and modules

The main functionalities required are reviewed hereafter.

3.1.1. Self-shielding treatment

The main goal is to provide available models and methods for all kind of reactors, flux spectra and isotopes. In order to provide better stability and enhanced accuracy, a continuous effort has been put into the improvement and development of self-shielding methods [5,21,22]. The main directions of research are improvement of the methodology (especially for Livolant-Jeanpierre method and Sub-group method), development of new models and elaboration of fine-multigroup reference calculations. These methods can be considered as the future basic method but will be improved to deal with all types of reactors.
Parallel computation should be available for the solver used within the self-shielding calculation and to manage the whole self-shielding step at the calculation scheme level.

3.1.2. Depletion solver

The depletion solver is a common module with Code_DARWIN3 [8,23,24] and it will also be coupled with Monte-Carlo calculations with TRIPOLI-4 [7,24]. It will be used to compute isotope depletion and production and for the calculation of core equilibrium fluxes at different burnup stages that can then be used in the production of the parameterized cross sections library. A continuous effort has been invested in the improvement of depletion methods, in its parallel implementation and in its uncertainties propagation.

3.1.3. Flux solvers

Steady-state solutions of the Boltzmann equation are used to study reactor behavior in normal operating conditions and carry out fuel management studies. Pin-by-pin calculations are intended to give further information on the local power peak, without having to apply fine flux reconstruction models.
Transport solvers, based on the classical collision probability method (PIJ), the TDT transport solver (MOC) [10,11,18], the discrete ordinates (IDT) solver[12,13] will treat 2D and 3D geometries and are already or will be implemented in APOLLO3.
A Finite Element Method solver called MINARET [14] has been implemented in APOLLO3 in order to perform 2D/3D transport SPN or SN calculation on unstructured meshes. The parallelization along the angular direction has been implemented using MPI library.
MINOS [25, 26] is a solver 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. In order to speed up calculations using a great number of meshes, an iterative domain decomposition method (IDD) has been implemented in the MINOS solver and will be extended to others methods [27].

3.1.4. Kinetic calculations

The APOLLO3 code should enable transient calculations with all flux solvers. All the kinetic parameters such as delayed neutron fractions will be provided for core transient calculations. All flux solvers will be adapted to kinetics calculation. At present, the method for kinetic calculations in APOLLO3 is implemented for MINOS solver with an implicit time step.

3.1.5. Sensitivity and uncertainties calculations

The main point is to provide models and methods to study the impact of different kinds of input data error and perturbations (such as nuclear data uncertainties, perturbation) on the results and safety parameters (criticality, reactivity coefficients, irradiated fuel isotopic composition, external source effectiveness, etc.). A continuous effort has been invested in the improvement of models and tools for sensitivity/uncertainty analysis and for propagating uncertainties. One solution based on generalized perturbation theory with adjoint neutron transport solution, will be available for all flux solvers. Sensitivity analysis and propagation models and methods will be implemented in order to predict changes in nuclide inventory and other parameters during depletion, due to perturbations in input data (nuclear data, initial nuclide abundancies…). Another solution is based on non-intrusive statistical methods. This kind of approach will be investigated too using URANIE tool [34].

3.1.6. Feedback effect, neutronic/thermal hydraulics coupling

The thermal-hydraulics of the core will be dealt with by a thermal-hydraulic code as FLICA4 [28] code coupled with APOLLO3 [35] via the SALOME platform [29] or specific API. For simple situations, APOLLO3 has its own simplified thermal-hydraulics model and this model will be extended to two-phases flows and other fluids as sodium. This code could be designed to manage coupling with other physical fields as thermal-mechanics: the PLEIADES [36,37] simulation platform for the study of the fuel design for any reactor concept with fuel rod code ALCYONE.

3.2. Architecture and internal data model (IDM)

An important objective is to perform reference calculation as well as project and industrial routine calculations with a code architecture that would allow an easy implementation of new methods and models for both lattice and core calculations. The goal of the new architecture design is to offer a toolbox for neutronic calculations based on a set of operators acting on shared objects (see figure 5). The user interface must be designed with a modular and dedicated structure consisting of a predefined set of operators or methods and a predefined set of objects (user data model, UDM). Figure 4 illustrates a prototype of this multi-level architecture that is enough versatile to be used by users interested by performing studies and analysis and also to be used by modelers interested by exploring their physic models or building new one. The aim of Internal Data Model (IDM) is to define shared concepts and data structures among the different components (see Figure 3). Moreover it defines the objects exchanged among the different solvers in order to transfer the information.

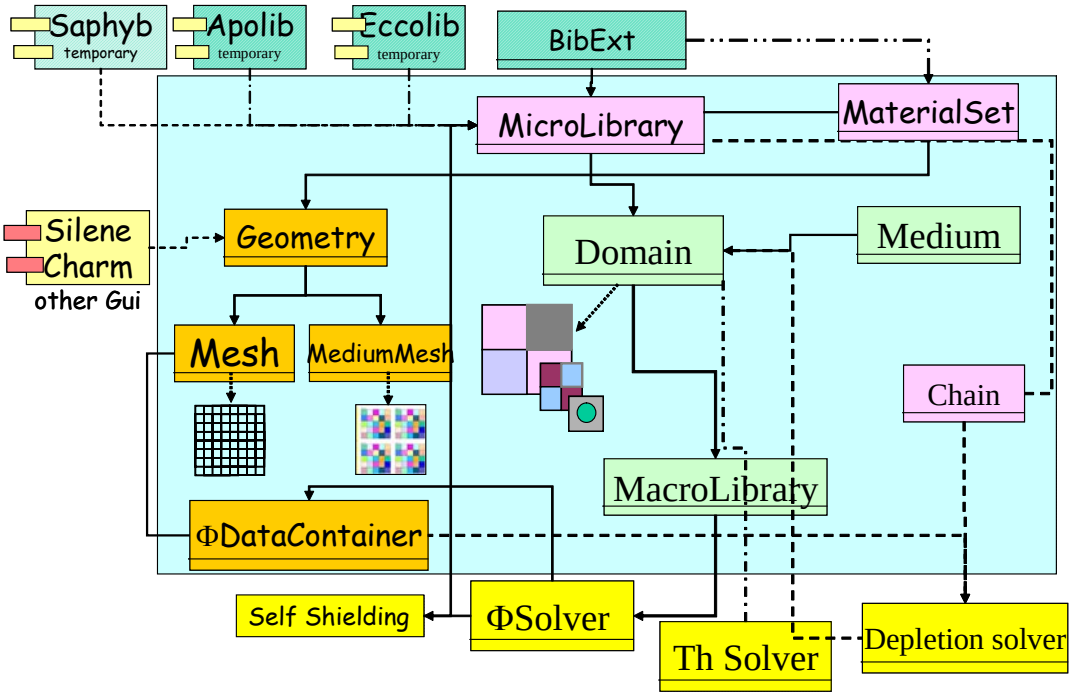


Figure 3. Internal Data Model (IDM) description

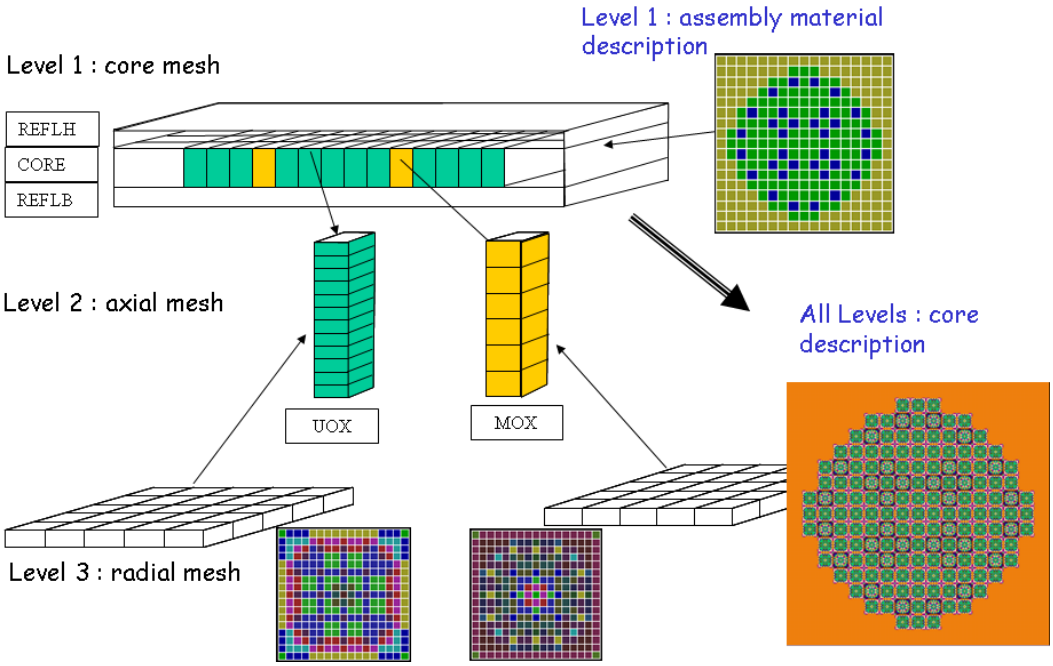


Figure 4. Multi level geometry principle

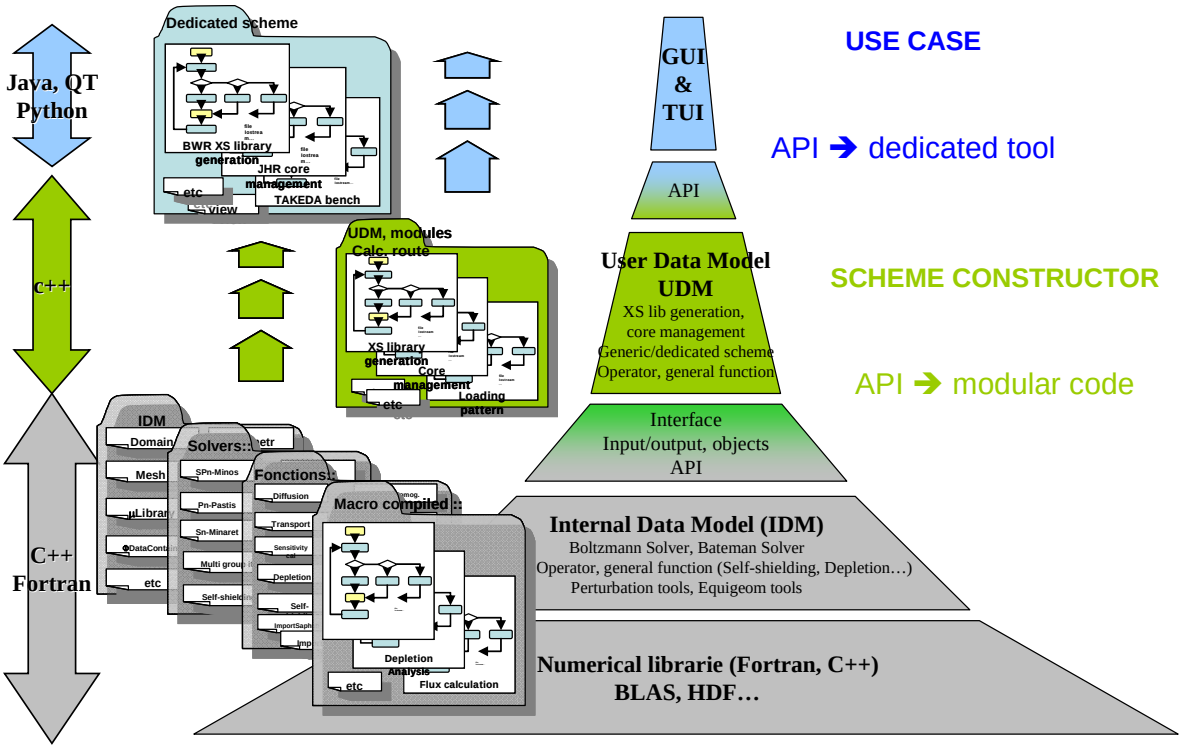


Figure 5. APOLLO3 architecture

3.3. Development process and quality insurance

All the development process is performed under quality assurance and follows a configuration management plan. SVN (Subversion) is used as Software Configuration Management tool: all the sources, documentation, makefiles, and V&V tests are managed. A non regression test cases base is under construction and the different versions of APOLLO3 are checked using this base on different platforms (Linux, Unix, Windows…).

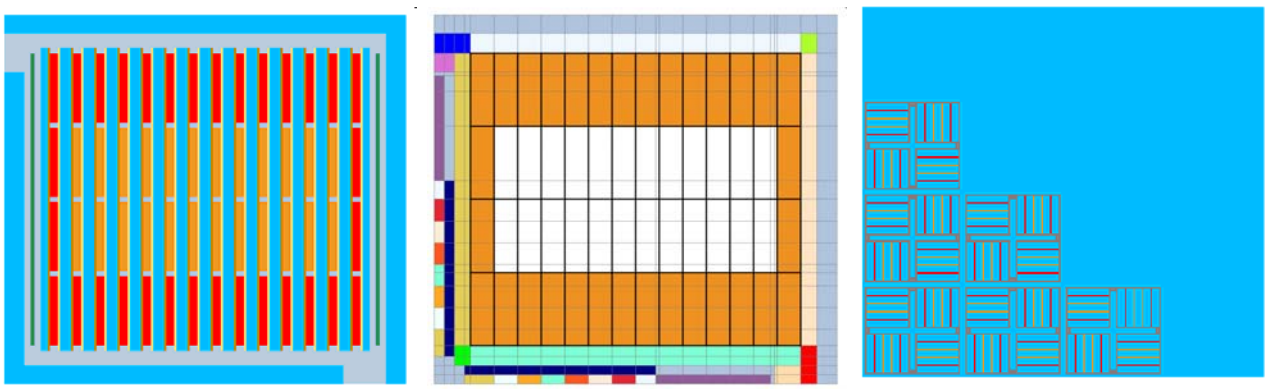
4. EXAMPLES OF USE CASES

To illustrate the new capabilities of APOLLO3 under development, we present briefly different use cases. The implementation of the first tests in order to verify and validate the different functionalities and the principles of the calculation routes is presented in the following sections.

4.1. LWR lattice and core calculation

The LWR test consists in enabling the main functionalities (assembly calculations, homogenization and condensation, 3D diffusion or SPn) and in testing the solver performances with a large number of regions and burnable media. The geometry of the core and the different steps of the calculation are illustrated in figure 6. This configuration is representative of a Material Test Reactor. The CPU time for a representative depletion calculation with 100 axial meshes (corresponding to 20 millions of regions and 2.4 millions of depletion media), and a

detailed isotopic depletion is around 700s with MINOS-diffusion and 2700s with MINOS-SP3: the memory requirement is around 38 Gb.



¼ of assembly
2D, 172 group, IDT
400 to 800 fuel depletion zones
per bundle

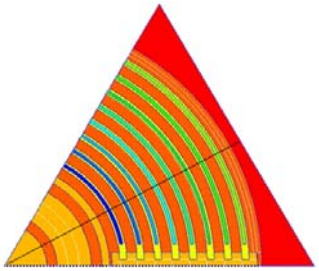
¼ of assembly
2D, 4 energy group
84 fuel depletion zones per bundle
120 to 130 homogeneous media

¼ of core (xy–plane)
3D calculation by MINOS
(diffusion or SPn)
3 to 20 millions of regions

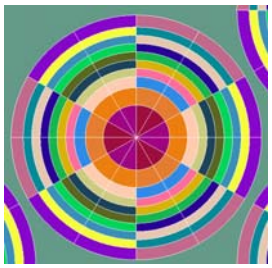
Figure 6. LWR lattice&core description

4.2. JHR core calculation

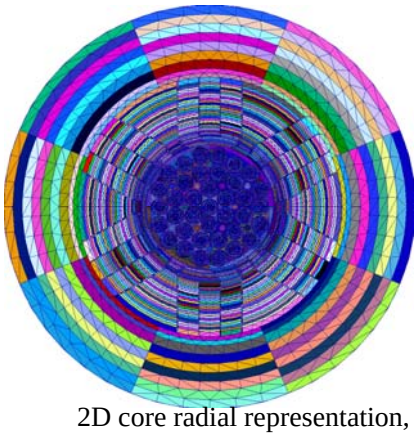
To first illustrate the capabilities of APOLLO3 to deal with 3D realistic complex configuration, JHR (Jules Horowitz Reactor) modeling and 3D core calculation have been achieved. Recent developments in APOLLO3 enable neutronic calculations dealing with very complex unstructured geometrical configurations. The discretization can be made either by using a very fine cartesian mesh and the fast simplified transport (SPN) solver MINOS, or by an automatic mesh generation based on triangles and the SN solver MINARET. Calculations have been performed both in sequential and parallel mode [27]. To illustrate these capabilities, we present an application on the future European research reactor JHR dedicated to technological irradiations in figure 7. The JHR core and assembly geometries are described via the Graphical User Interface SILENE [30]. The results of the 2D calculations are reported in table 1. The results are compared with those obtained by Monte Carlo calculations with the Tripoli4 code and a point-wise description of the cross sections producing a 1σ standard deviation of 30 pcm. The CPU time is nearly proportional to the number of mesh points with respect to 2D calculations. Table 1 shows the efficiency of the domain decomposition method on a parallel computer. Table 2 refers to the very first 3D calculation performed with a grid discretization of 1000x1000x42 mesh and the MINOS solver for the sequential version as well as with a parallel calculation and with MINARET transport solver with P1 spatial approximation and S4 discrete ordinate discretization. Further investigation will be conducted with regard to the reactivity discrepancy.



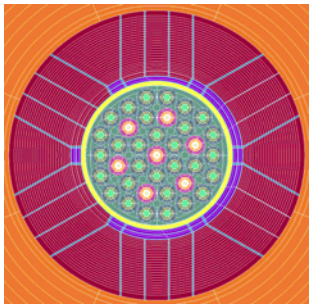
Assembly radial geometry of transport calculation



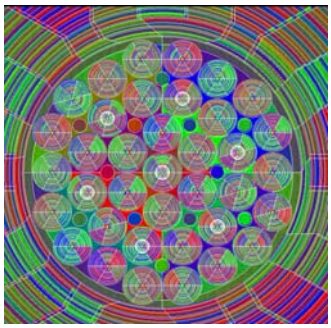
Neutronics modeling of a JHR assembly, homogenized in 20 regions and collapsed in 6 energy

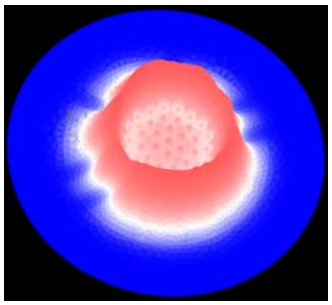


2D core radial representation, calculation by MINARET 4149 regions, 40112 triangles



Core radial representation, 3D calculation by MINOS (diffusion or SPn), 42 axial planes, 42 million regions





Core radial representation, 3D calculation by MINARET (diffusion or SN), 42 axial planes, 1.68 million triangles Flux distribution

Figure 7. JHR application : different levels of geometrical representation and flux distribution

Table 1. 2D JHR results : reactivity and CPU time

Case	Keff	Δρ / ref	CPU in s
TRIPOLI-4	1.31239	-	
MINOS SP1	1.30717	-398	1490
MINOS SP7	1.31141	-74	4370
MINOS SP1 with 8 subdomains (8 procs)	1.30717	-398	165
MINOS SP1 with 36 subdomains (36 procs)	1.30717	-398	34
MINARET (Diff)	1.30808	-328	145
MINARET (Transp. S4)	1.31305	+50	2109

MINARET (Transp. S8)		1.31314	+57	3850
MINARET (Transp. S4) parallelization along the angular direction	**Nb proc 1**	1.31305	+50	2109
	Nb proc 2			1133
	Nb proc 4			580

Table 2. 3D JHR results, 42 axial planes : reactivity and CPU time

Case		**Keff**	**CPU in s**
MINOS SP1 (grid 1000x1000x42)	**Nb proc 1**	1.13587	36510
	Nb proc 4		11955
	Nb proc 6		8900
MINARET (Transp. S4P1) parallelization along the angular direction	**Nb proc 1**	1. 11784	50425
	Nb proc 4		13870

4.3. Hexagonal benchmark with APOLLO3

A recent development allows treating 3D hexagonal geometries using very fast SPN calculation (MINOS Solver, [38]). To illustrate the new hexagonal capability of MINOS, we present the results obtained on the small FBR core proposed by T. Takeda and H. Ikeda [31]. In table 3, the MINOS calculations are carried out with different degrees of approximation on the flux and with a splitting of each hexagon into four trapezoid (M1). These results are very close to those obtained with the CRONOS code using a splitting of hexagons into 6 triangles (M1) or into 54 triangles (M3) and a linear (d°1) or parabolic (d°2) or cubic (d°3) or fourth order (d°4) approximation on the flux. Figure 8 presents the MINOS geometry and the power map for the middle plane of the benchmark.. Table 3 shows the efficiency of the Minos solver in APOLLO3.

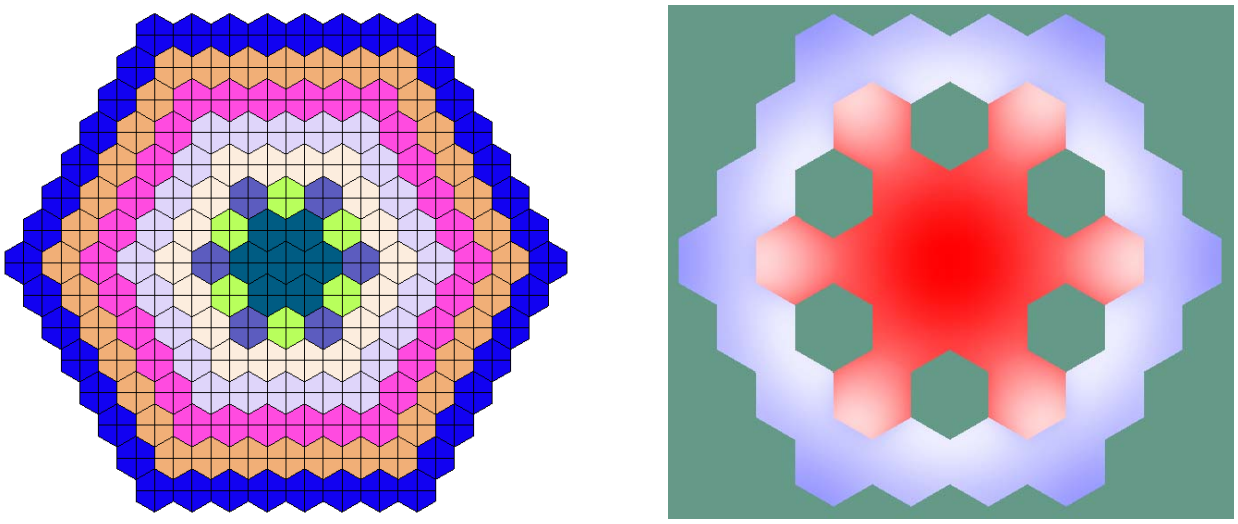


Figure 8. The MINOS mesh and the computed power for the middle plane of the 3D Takeda4 benchmark

Table 3. MINOS and CRONOS results for the 3D Takeda4 benchmark

*convergence obtained	Keff	CPU time (s)
Minos M1 d° 1	1.06966	9.9
Minos M1 d° 2	1.07251	52.9
Minos M1 d° 3	1.07248	166.3
Minos M1 d° 4*	1.07249	312.0
Cronos M3 d° 2*	1.07249	634.7

4.4. Other cases with APOLLO3

An optimization of the loading pattern using evolutionary algorithms has been performed with success with APOLLO3 code [32]. Other tests will be selected including LWR, HTR and SFR configurations using a 2D/3D transport calculations with perturbations theory, generation of multi-parameter cross section library, SFR&JHR calculations with thermal-hydraulic coupling, transient conditions…

5. V&V&Q PROCESS

The objectives of the V&V&Q (Verification, Validation, Qualification) process is to provide the users with a validated code package, qualified on integral experiments, to check that the errors (ie the average discrepancies on given integral parameters such as critical masses or pin-by-pin power distributions) and «calibrated» in a specified range of problems are lower than the target accuracy. The strength of CEA approach is to use a complete library/code package including

GALILEE library generation tool and the TRIPOLI continuous energy Monte-Carlo code. One can distinguish different steps:

- The first step of the V&V&Q process verifies that the numerical resolution of neutronics models and programming of each module are correct. This verification is also based on a dedicated “Test Machine” which avoids regression in the new code versions.
- The second step corresponds to the numerical Validation, which quantifies the accuracy of the neutronics models used in APOLLO3. The APOLLO3 Validation is carried out both on functionalities (Pij, resonance self-shielding, depletion, MOC, Sn, Pn solvers,…) and on a reference calculation scheme. Generally, this validation is based on the comparison of APOLLO3 deterministic calculation against TRIPOLI4 continuous-energy Monte Carlo reference calculation. Both calculations use the same nuclear data library (based on JEFF3.1 evaluation). The APOLLO3-TRIPOLI4 comparison is performed on numerical benchmarks, representative of PWR, BWR, GFR, SFR, JHR problems.
- The Qualification also called "physical validation" is the third step, corresponding to the comparison of the results of the global package (code + reference calculation scheme + nuclear data library) with experimental results from integral measurements.

A first set of experiments characterized by their fundamental measurements are used to qualify the nuclear data (and the corresponding multi-group library) for the main isotopes: material bucklings, actinide fission rate ratios, conversion factors, etc. are measured in the EOLE and MASURCA reactors [33]. Capture cross sections of the main poisoning Fission Products, separated actinides, absorbers isotopes are qualified through reactivity worth measurement of samples by an oscillation technique in various spectra in the MINERVE zero power reactor [33].

A second set of mock-up experiments are used to qualify the calculation of every reactor parameter. From this qualification process, based on several hundreds of integral measurements, an Uncertainty Quantification is carried out: the scaling: the scaling factor (ie the a posteriori C/E reduction using representativity factor) for each design parameter, as well the associated uncertainty, is obtained for the APOLLO3 product.

Some parts of the validation process can be envisaged to analyze and validate the evolving code versions during the period 2012-2015. Since the user interface is available, a collection of tests and benchmarks can be easily defined and a large number of comparisons with Monte Carlo calculations could be carried out to validate APOLLO3 for a wide range of applications.

6. CONCLUSION

APOLLO3, a new generation code system for neutronic applications, has been presented in this paper. The main objectives of this development project are to renew current deterministic codes, to overcome current methodology limits like the two-step calculation approach (lattice followed by core calculations) and to extend fine resolution methods like MOC to whole 3D core simulations. Current developments mainly focus on LWR and FR reactors, but many axes of development are in progress, like advanced lattice solvers, parallelization and functionalities for various types of reactors.

APOLLO3 is under development and an important work must be done to supply to users a validated code package, qualified on integral experiments, to check that the errors «calibrated» in a specified range of problems are lower than the target accuracy on well defined integral parameters. Comprehensive benchmarking and validation against Monte-Carlo calculations must be done.

Nevertheless, the APOLLO3 version under development has demonstrated with preliminary applications a good potential to overcome the limitation of the two-step approach currently used for power reactors and constitutes a powerful code system for power reactor analysis (PWR, BWR, GFR, SFR…) with rectangular and hexagonal fuel arrangement, as well as for naval propulsion reactors and for experimental and research reactors.

The key milestones for the APOLLO3 project are :

- APOLLO3 “2010 release” to implement the current “calculational routes” based on APOLLO2, CRONOS, and ERANOS codes and to have the capability to easily connect to the other software components DARWIN, GALILEE and TRIPOLI,
- APOLLO3 “2012 release” to perform advanced design studies of GEN-IV reactors and as reference 3D core code for LWR applications. It will be used to perform detailed design studies for the SFR prototype;
- APOLLO3 “2015 release” for the industrial and multi-generation applications and subsequent integration in AREVA and EDF industrial calculation platforms. It will be used for detailed design studies of GEN-IV reactors and as reference 3D core code.

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