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HORUS3D/N NEUTRON CALCULATION TOOL, A DETERMINISTIC SCHEME DEDICATED TO JHR DESIGN AND SAFETY STUDIES

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Abstract

The international Jules Horowitz Material Testing Reactor (JHR) is under construction at CEA Cadarache research center, in southern France. Its first criticality is foreseen by the beginning of the next decade. In order to perform JHR neutron simulations, a specific calculation scheme, named HORUS3D/N (Horowitz Reactor simulation Unified System 3-Dimension/Neutron), was developed since the 2000's for the very first JHR definition studies. Then, it was improved and modified in parallel with the JHR design evolution, integrating the most accurate neutron codes and nuclear data libraries. This paper describes the very latest version of HORUS3D/N, named HORUS3D/N v4.2. The industrial route is based on APOLLO2.8-4 and CRONOS2.10 deterministic codes, and the European nuclear data library JEFF3.1.1. Besides, HORUS3D/N v4.2 includes the APOLLO2.8/REL2005/CEA2005 package recommendations applied for light reactor studies. The paper provides also the performance quantification of HORUS3D/N v4.2 as a result of the Verification & Validation – Uncertainty Quantification process (or V&V-UQ process). This reference calculation scheme is now a basis for the development of the neutron calculation tool dedicated to JHR operation and loading studies.

Key Words: JHR, HORUS3D/N, neutronics

I. INTRODUCTION

The Jules Horowitz Reactor (JHR) [1] is the future Material Testing Reactor under construction in southern France. It will be a major research infrastructure in Europe, designed to support existing power plant operations and lifetime extension, as well as future reactor design. Its objectives are to test the new structural material and fuel behavior under irradiation for the development of the GEN-III and GEN-IV reactors, and to demonstrate the satisfactory stainless steel behavior for current French Pressurized Water Reactor (PWR) lifetime extension. The JHR will also supply 25% to 50% of the European demand for radio-isotopes, mainly ^{99}Mo , for medical applications [2]. The JHR first criticality is foreseen by the beginning of the next decade.

The JHR design and safety studies have been carried out using a neutron calculation scheme named HORUS3D/N (Horowitz Reactor simulation Unified System 3-Dimension/Neutron). HORUS3D/N was developed since the 2000's to meet the specific needs of JHR [3], [4], [5].

In this paper, after a brief description of JHR, the HORUS3D/N v4.2 calculation package will be presented. It will then focus on the assessment of the biases and uncertainties associated with HORUS3D/N v4.2 industrial route computations, as a result of the Verification & Validation - Uncertainty Quantification process (or V&V-UQ process).

II. THE JULES HOROWITZ REACTOR

The JHR is a tank-in-pool type reactor using light water as its coolant and moderator, with a maximum thermal power of 100 MW [1]. The reactor will start with a standard density low enriched U_3Si_2 fuel (e% ^{235}U = 19.75%, density 4.8 g.cm^{-3}), and a 70 MW thermal power. It will operate with a cold fuel (fuel temperature~100°C) and a slightly pressurized light water

(mean pressure: 8 bars; inlet temperature: 30°C; flow rate: 7400 m³/h). The core can be loaded with 34 to 37 fuel elements, inserted in an aluminum alloy rack (see Fig.1). In order to reach a high fast neutron flux level in the core ($\sim 5 \times 10^{14}$ n/cm²/s), the fuel elements (see Fig.2) are made of 3 sets of 8 curved plates assembled with aluminum stiffeners and clad with Al-Fe-Ni. A boron insert is positioned 1 cm above the active height in each plate to prevent nucleate boiling departure at the top of the core water channels. A hafnium control rod, connected to an aluminum follower (the follower is an aluminum tube replacing the absorber part of the control rod when it is withdrawn) can be loaded in the central hole of the fuel assembly. The core area is surrounded by a reflector made of beryllium blocks which optimizes the core cycle length and provides intense thermal fluxes in this area ($\sim 5 \times 10^{14}$ n/cm²/s).

Up to 20 experimental devices can be loaded and irradiated at the same time (see Fig.1), either in the core (in the cells of the rack or in the central hole of the fuel elements), or in the reflector (in static locations or on displacement systems in order to investigate transient regimes occurring in accidental situations).

This flexible experimental capability can create up to 16 dpa/year for in-core material experiments (to be compared to the 2-3 dpa/year produced in industrial Light Water Reactors), and 600 W.cm⁻¹ for 1% ²³⁵U enriched fuel sample experiments in reflector, with 260 full power operation days per year.

III. THE HORUS3D/N v4.2 NEUTRON CALCULATION PACKAGE

The JHR innovative characteristics led to the development of a specific neutron calculation scheme called HORUS3D/N. This computation tool was developed since the 2000's for the needs of the very first JHR definition studies [3]. Then it was improved and modified in

parallel with the JHR design evolution (see Fig.3), integrating the most accurate neutron codes and nuclear data libraries [4], [5].

The HORUS3D/N v4.2 package is composed of 3 different routes (see Fig.4) which include the JEFF3.1.1 European nuclear data library [6]:

- an industrial route based on a two-step APOLLO2.8-4 [7] /CRONOS2.10 [8] deterministic calculation scheme (see § III.A). In the first step, for each kind of components present in the JHR, the 2D APOLLO2 lattice code, using fine energy-meshing, provides libraries of self-shielded cross sections collapsed into 6 energy groups and tabulated versus burnup (or fluence). In the second step, these collapsed cross sections are introduced into a 3D full core calculation performed with the CRONOS2 diffusion code on a hexagonal spatial meshing,
- two reference routes for validation purposes:
 - a reference route for the JHR beginning of life core calculations (at time-step 0), based on 2D and 3D continuous-energy Monte Carlo TRIPOLI-4.9® computations [9], on heterogeneous geometry (see § III.C),
 - a deterministic reference route for the JHR core calculations during depletion, based on 2D APOLLO2.8-4-MOC computations [10], [11], on heterogeneous geometry (see § III.B).

The goal of HORUS3D/N industrial route simulations is to predict within a limited time¹, neutron parameters (reactivity, power distribution, control rod reactivity worth, etc.), with quantifiable confidence, across the JHR operating domain (see Table I), and for different time

¹ 2 hours for depleted 3D full core up to 82 GWd/t_{HM}, corresponding to the mean end-of-cycle burn-up of the JHR core.

steps: beginning of cycle, Xenon equilibrium, mid cycle, end of cycle. Therefore, the HORUS3D/N industrial scheme was submitted to the rigorous Verification & Validation - Uncertainty Quantification process (or V&V-UQ process), by comparing, in particular, the industrial deterministic scheme with the two reference routes mentioned above (see § IV).

Table I
JHR operation domain

Fuel assembly load in the aluminum alloy rack	Maximal experimental load	
	<i>In core</i>	<i>In reflector</i>
34 to 37 fuel assemblies with or without Hafnium control rods	7 fuel elements with experiments + 3 cells loaded with experiments	12 experiments

III.A Industrial route calculation scheme

III.A.1 APOLLO2 first step

Concerning the APOLLO2 first step of the HORUS3D/N v4.2 industrial route (see Fig.4), the main computation options follows the APOLLO2.8/REL2005/CEA2005 package recommendations developed by CEA light water reactor studies (see Table II) [12]. For the fuel assembly computations, they are the following:

- concerning the self-shielding computations:
 - the SHEM-281 group energy mesh is included in the calculations; this fine energy meshing below 23 eV prevents resonance self-shielding approximations for all isotopes [13],
 - the resonant mixture self-shielding treatment is applied for the U₃Si₂-Al fuel (²³⁵U, ²³⁸U, ²³⁹Pu and ²⁴⁰Pu) up to 200 eV intermediate range, and for the Hafnium absorber (¹⁷⁷Hf, ¹⁷⁹Hf, ¹⁷⁶Hf, ¹⁷⁸Hf, ¹⁸⁰Hf) up to 1keV, in order to rigorously account for resonance overlap of these major actinides and isotopes in these energy ranges,

- the computations are performed on 1 D cylindrical simplified geometry,
- concerning the flux computations:
 - the spatial meshing of the fuel assembly is performed with 24 angular sectors, i.e. 4 angular sectors on $1/6^{\text{th}}$ of the assembly (see Fig.5), allowing for an accurate assessment of the azimuthal thermal flux gradient near the stiffeners,
 - the computations are performed using the APOLLO2 Method Of Characteristics (MOC) flux solver with the SHEM-281 group energy mesh (no collapsing), at time-step zero and in depletion,
 - the calculations are based on fine tracking values:
 - Tracking step: $\Delta R=0.04\text{cm}$
 - Radial direction number in $[0, \pi]$: $N\Phi=24$
 - Polar direction number in $[0, \pi/2]$: $N\Psi=3$ (Bickley quadrature)
 - Associated with a P3 Legendre polynomial expansion for anisotropy scattering
 - the homogeneous B1 model with research of critical buckling is considered for the neutron leakage modelling.

The self-shielding and the flux is computed at the following burn-up values (in MWd/t): 0, 37.5, 75.0, 112.5, 150, 325, 500, 750, 1000, 1500, 2000, 2500, 3000, 4000, 6000, 8000 + every 4000 MWd/t up to 150 GWd/t.

This first calculation step provides self-shielded and depleted cross sections collapsed into 6 energy groups, input data for the CRONOS2 second step computation (see § III.A.2).

Table II
Industrial route - APOLLO2 computation options - 2D fuel clusters/reflectors

<i>APOLLO2 computation options – 2D fuel clusters/reflectors</i>		HORUS3D/N v4.2
APOLLO2	version	APOLLO2.8-4
Library	version	JEFF3.1.1 (CEAV5.1.2, processed for APOLLO2)
Self-shielding	energy mesh	SHEM - 281 groups
	method	Livolant-Jeanpierre + resonant mixture
	geometry	1D Cylindrical for most of the cases
Flux calculation	energy mesh (collapsed cross sections)	SHEM (281 g) <i>Except for:</i> - radial reflector: 22 g (t0 only) ⁽¹⁾
	geometry	1/6 th of the fuel assembly with or without environment, “RZ” assembly for the axial reflector
	spatial mesh	24 angular sectors
	solver	MOC (2D) <i>Except for:</i> - axial reflector: SN
	Anisotropic scattering	P3
	tracking	cyclic
	Fine tracking values	- Tracking step: $\Delta R = 0.04$ cm - Radial direction number in $[0, \pi]$: $N\Phi = 24$ - Polar direction number in $[0, \pi/2]$: $N\Psi = 3$ - Polar quadrature: "Bickley"
	neutron leakage: homogeneous B1 model	critical buckling

(¹) obtained from the 2D core computations (see § III.B) with homogenized fuel assemblies.

III.A.2 CRONOS2 second step

Concerning the second step of the HORUS3D/N v4.2 industrial route (see Fig.4), the 3D full core calculations are performed with the CRONOS2 diffusion code, using 6 energy groups associated with transport-diffusion equivalence factors, on a hexagonal spatial meshing [4]. Despite the apparently irregular location of the fuel element in the core, the assembly pattern has a hexagonal macro-symmetry (see Fig.6). With the iso-parametric finite element method in the CRONOS2 code, each hexagonal mesh cell can be considered as a “Super Finite Element” (SFE). These SFEs need a conform mesh of arbitrary triangles, which form the basic finite elements. The fuel elements are meshed with dodecagons. The reflector region is modeled with a

series of particular SFEs, allowing for an accurate modeling of radial and azimuthal heterogeneities. A macroscopic depletion calculation is used in HORUS3D/N. The evolution of heavy nuclide content (^{235}U , ^{238}U , ^{239}Pu) is thus estimated by data interpolations from 2D APOLLO2 infinite lattice computations at the considered burnup value. Only ^{10}B , ^{135}Xe and ^{149}Sm isotopic contents are calculated directly by CRONOS2. An optimal time mesh has been determined in order to follow the evolution of these isotopes and the 3D spatial burn-up variations.

III.B APOLLO2 reference route in depletion

The APOLLO2-MOC reference route (see Fig.4) follows, as the first step of the industrial route (see III.A), the same APOLLO2.8/REL2005/CEA2005 package recommendations [12] (see Table III): the use of the SHEM-281 group energy mesh, the resonant mixture self-shielding treatment for the $\text{U}_3\text{Si}_2\text{-Al}$ fuel and for the Hafnium absorber, fine tracking values associated with a P3 Legendre polynomial expansion for anisotropy scattering. Moreover, the spatial meshing of the assembly (12 angular sectors) and of the reflector were refined and optimized (i.e. they correspond to the most computation time accuracy compromise) (see Fig.7 and Fig.8), thanks to the introduction into HORUS3D/N of the SALOME platform [14], a modern and high performance pre-processing user interface which generates a meshing in a few minutes compared to weeks with former tools.

Thanks to SALOME, the spatial meshing of the reflector was upgraded (see Fig.8) in order to:

- refine the radial meshing near the core in order to respect the thermal neutron flux gradient,

- define a specific meshing for each experiment (without changing the meshing of the rest of the reflector),
- define the meshing which corresponds to the most computation time accuracy compromise.

Table III
Reference route - APOLLO2-MOC computation options - 2D core

<i>APOLLO2-MOC computation options – 2D core</i>		HORUS3D/N v4.2
APOLLO2	version	APOLLO2.8-4
Library	version	JEFF3.1.1 (CEAV5.1.2)
Self-shielding	energy mesh	SHEM - 281 groups
	method	Livolant-Jeanpierre + resonant mixture
	geometry	1D Cylindrical for most of the cases
Flux calculation	energy mesh (collapsed cross sections)	22 g (collapsed from Pij 1D calculation)
	geometry	2D core
	spatial mesh	Assembly: 12 angular sectors Reflector: optimized spatial mesh
	solver	MOC
	Anisotropic scattering	P3
	tracking	Non cycling
	Fine tracking values	- Tracking step: $\Delta R = 0.04$ cm - radial direction number in $[0, \pi]$: $N\Phi = 24$ - polar direction number in $[0, \pi/2]$: $N\Psi = 3$ - polar quadrature: "Bickley"
	Leakage	Axial buckling No axial leakage when compared with TRIPOLI4 or CRONOS2

III.C TRIPOLI4 Reference route calculation route at time-step 0

The TRIPOLI-4.9® code is a 3-Dimensional continuous energy computer code for particle transport [9]. It is used to solve the integral Boltzmann equation for neutrons, with the Monte Carlo method. The code uses PENDF format continuous energy cross-sections and probability tables, from the international evaluations JEFF3.1.1. The detailed JHR geometry was

described on the basis of to-be-built plans and material balance of the different core elements (rack, JHR assemblies, etc) provided by the manufacturers. The JHR 3D quasi-exact geometry is modeled with a surface-based geometry in the TRIPOLI-4® code (see Fig.1).

IV. HORUS3D/Nv4.2 INDUSTRIAL ROUTE PERFORMANCE QUANTIFICATION

The HORUS3D/N simulations are used to predict neutron parameters with quantifiable confidence across the JHR application domain. Therefore, the HORUS3D/N development followed the rigorous Verification & Validation - Uncertainty Quantification process (or V&V-UQ process) [5]. First, it was submitted to a Verification step including non-regression tests, and then to a Validation process in order to Quantify the biases and Uncertainties to be applied to each parameter computed with the calculation route. These biases and uncertainties have two origins:

- the nuclear data which are physical parameters input and which describe all the interactions between neutrons with matter (see § IV.A),
- the models, and more generally, all the approximations used in the APOLLO2/CRONOS2 calculation scheme (approximation of the real geometry, energy meshing, resonance self-shielding, depletion, flux solver, etc.) (see § IV.B).

IV.A Nuclear data validation

In order to provide JHR representative measurement data, the AMMON program was launched between late 2010 and early 2013 in the EOLE zero-power critical mock-up [15]. The AMMON experiment consisted of an experimental zone dedicated to the analysis of the JHR neutron and photon physics surrounded by a driver zone. The experimental zone, for the

reference configuration, contained 7 JHR fresh fuel standard assemblies-like (see § II) inserted in an aluminum alloy hexagonal rack (30 cm side length). The driver zone for the reference configuration consisted of 622 standard Pressurized Water Reactor (PWR) fuel pins (3.7% ^{235}U enriched UO_2), with Zircaloy-4 cladding and stainless steel overcladding. The hexagonal lattice pitch of the driver pins was optimized in order to reproduce, as well as possible, the same neutron spectrum as the one of the experimental zone. 5 configurations were studied (see Fig.9):

- a reference configuration with 7 JHR fresh fuel assemblies,
- a configuration with a hafnium control rod totally or half inserted in the central assembly,
- a configuration with a beryllium block replacing the central assembly,
- a configuration with water in the middle of the central assembly (withdrawn Hf rod follower),
- a configuration with water replacing the central assemblies.

The interpretation of the AMMON experiments with reference TRIPOLI-4[®] calculations using the JEFF3.1.1 nuclear data library, made it possible to assess the biases and uncertainties originating from the nuclear data². These results were transposed from the AMMON experiment to the real JHR core with the representativity methodology [16] [17], for the JHR-Beginning Of Life but also for the JHR in equilibrium. Indeed, a specific study showed that the ^{239}Pu (produced in the $\text{U}_3\text{Si}_2\text{-Al}$ fuel thanks to ^{238}U radiative capture) contribution in assembly fission rates remained limited (<10%) compared to the ^{235}U contribution during the JHR lifetime (the JHR neutron spectrum can then be considered as constant). Thus, even if the AMMON experiments were performed on fresh JHR fuel, the results could also be transposed to the JHR in equilibrium.

² Few physical assumptions are made in TRIPOLI-4[®] that is why the biases are supposed to come only from nuclear data.

The biases and uncertainties on the different neutron parameters computed with HORUS3D/N originating from the nuclear data are summarized in [15]. They are not recalled here. Only the results of the global validation step are presented in § IV.C.

IV.B Scheme validation

An important validation step was carried out by comparing the deterministic calculations with reference ones:

- on the fuel assembly clusters (see § IV.B.1),
- on the full core (§ IV.B.2).

IV.B.1 Fuel assembly APOLLO2 scheme

The validation of the APOLLO2 assembly scheme was carried out on the 2 main fuel clusters: the fuel assembly with the Al follower and the fuel assembly with the Hf rod. It consisted in comparing the APOLLO2 results with the Monte Carlo TRIPOLI-4[®] computations at step 0 with the same JEFF3.1.1 library.

Different computations were compared: reactivity (considering the k_{∞} breakdown into the 6 Fermi factors), fuel fission and absorption rates per fuel plate, hafnium rod efficiency (considering each of the 281 groups for the main isotopes). The main results of the validation step are the following at step 0:

- the reactivity is overestimated by $\sim +30$ pcm for the fuel assembly with the Al follower,
- the hafnium rod efficiency is overestimated by +1.1%,
- the discrepancy of the fission rate per fuel plate is less than 0.4%.

These very good results validated the APOLLO2 assembly scheme.

This first validation step ensures that the fuel assembly scheme only add a limited bias in the core validation step.

IV.B.2 Full core APOLLO2/CRONOS2 scheme

In order to assess the biases and uncertainties due to the calculation scheme of HORUS3D/N v4.2 industrial route, the validation step was carried out by comparing the deterministic calculations with reference route calculations (see Fig.4):

- 2D and 3D continuous-energy Monte Carlo TRIPOLI-4® calculations, for the JHR beginning of life core calculations,
- 2D APOLLO2-MOC deterministic calculations, for the JHR depleted core calculations (such as the equilibrium core for example).

Over 100 validation cases were performed to cover the JHR operation domain and to ensure statistical representativeness [5].

The detail of this study is not presented in this paper. Only the results of the global validation step are presented in § IV.C. Nevertheless, as an example, Fig.10 illustrates the scheme bias and uncertainty (2σ) calculation methodology considering reactivity at step 0 for core configurations when control rods are inserted. The X axis represents the configuration numbering used, and the Y axis the reactivity discrepancy between APOLLO2/CRONOS2 and TRIPOLI-4® computations. The bias corresponds to the mean value of the discrepancies. The uncertainty at 1σ is then the average deviation to this mean value. We checked that 95% of the results were in the expected $\pm 2\sigma$ interval.

IV.C HORUS3D/N v4.2 biases and uncertainties

The results of the validation steps (see § IV.A and § IV.B) were combined as follows for each JHR relevant parameter computed with the HORUS3D/N industrial route, assuming the decorrelation between the two biases and uncertainties origins: the nuclear data and the numerical scheme:

- Biases:
$$\text{Biases}_{Global} = \text{Biases}_{scheme} + \text{Biases}_{ND} \quad (1)$$

- Uncertainties:
$$\sigma_{Global} = \sqrt{\sigma_{scheme}^2 + \sigma_{ND}^2} \quad (2)$$

With:

- Biases_{scheme} : biases of HORUS3D/N due to the calculation scheme,
- Biases_{ND} : biases of HORUS3D/N due to Nuclear data,
- σ_{scheme} : uncertainties of HORUS3D/N due to the calculation scheme,
- σ_{ND} : uncertainties of HORUS3D/N due to Nuclear data.

Table IV summarizes the results of the validation of HORUS3D/N v4.2 industrial route.

Table IV
HORUS3D/N v4.2 industrial route biases and uncertainties assessment

HORUS3D/N v4.2 industrial route		Bias and uncertainties (2σ)	
		Step 0	Evolution
Starting core reactivity		-862 pcm ± 640 pcm	-
Reactivity of a critical core at nominal and cold conditions (pcm)	Without Hf rod	-71 pcm ± 650 pcm	-233 pcm ± 827 pcm
	With Hf rods	-343 pcm ± 791 pcm	-663 pcm ± 911 pcm
Xenon equilibrium antireactivity		-	+0% ± 3.2%
Xenon antireactivity at the peak		-	+0% ± 16.9%
Samarium antireactivity		-	+0% ± 2.5%
Integral Hf rod worth		+5,9% ± 4,7%	+4.6% ± 4.7%
Differential Hf rod worth		+4,3% ± 3,2%	+8.9% ± 3.2%
In core experiment reactivity worth		-1,5% ± 6%	-3.4% ± 6.1%
In reflector experiment reactivity worth		-72 pcm ± 39 pcm	-92 pcm ± 31 pcm
Radial power distribution - Assembly level		+0% ± 5,4%	+0% ± 5.4%
Radial power distribution - Plate level (int)		+0% ± 8,2%	-0.7% ± 8.8%
Radial power distribution - Plate level (ext)			+1.2% ± 11.3%
Hot plate power		-2,6% ± 4,6%	-2.6% ± 4.6%
Axial power peaking factor (step 0)		+2,5% ± 6,3%	-
Burunp distribution - Assembly level		-	+0% ± 4.1%

V. CONCLUSIONS

The HORUS3D/N calculation scheme, dedicated to JHR neutron simulations, was developed since the 2000's for the needs of the very first JHR definition studies. Then it was improved and modified in parallel with the JHR design evolution, integrating the most accurate neutron codes and nuclear data libraries, and recommendations applied for light reactor studies.

The very latest version of the scheme, HORUS3D/N v4.2, presented in this paper, is now a basis for the development of the neutron deterministic calculation tool dedicated to JHR operation and loading studies [18]. This new tool will have to deal with time constraint - a JHR loading will have to be fully calculated in a few hours, and user experience - the studies will be performed routinely by JHR operators.

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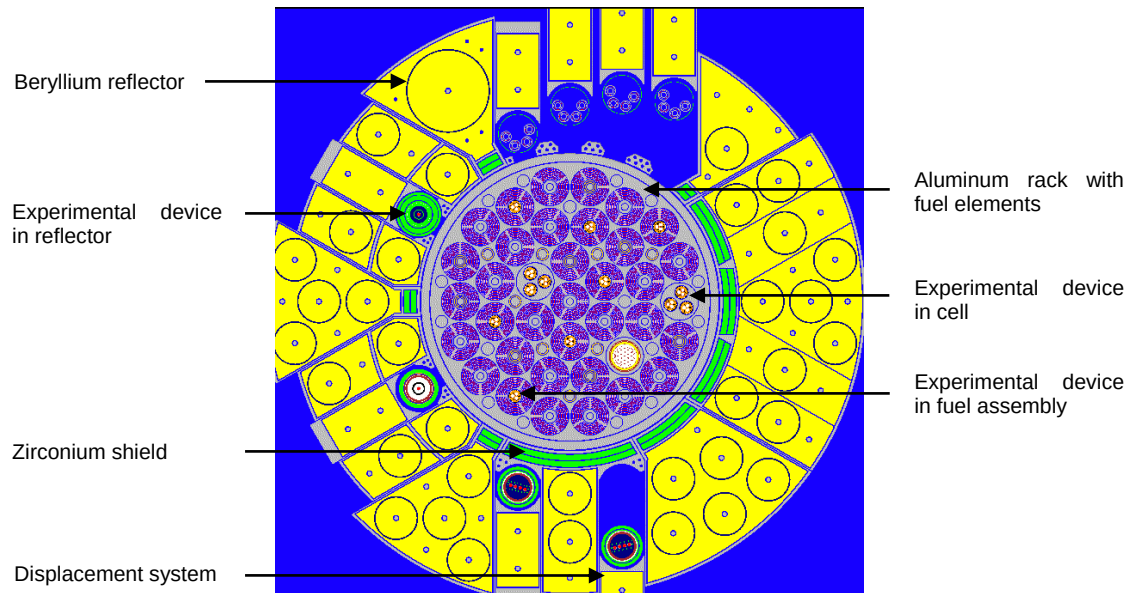


Fig.1. JHR core description

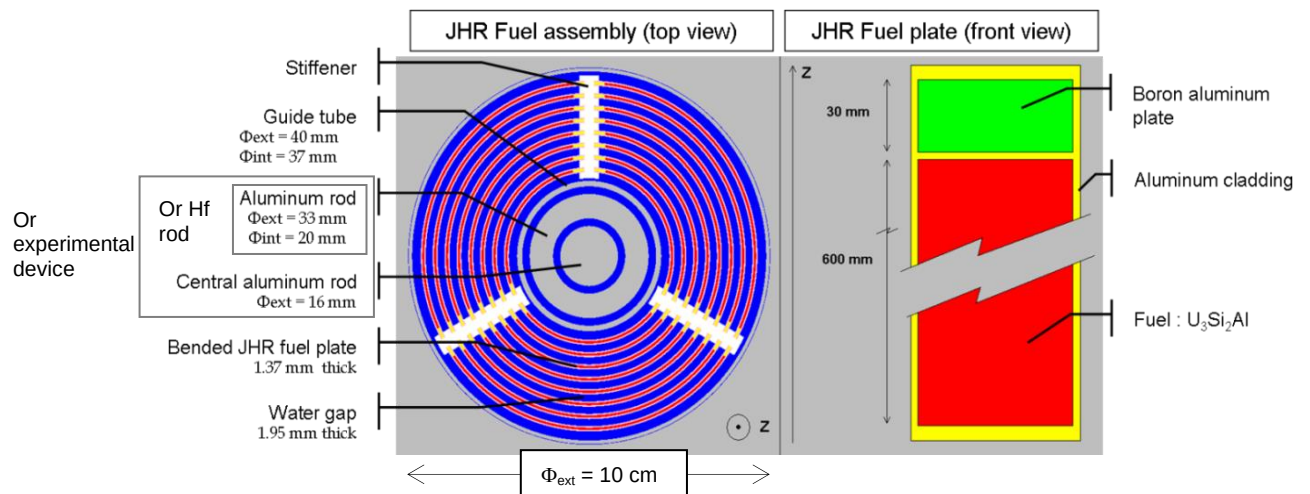


Fig.2. JHR fuel element and JHR fuel plate description

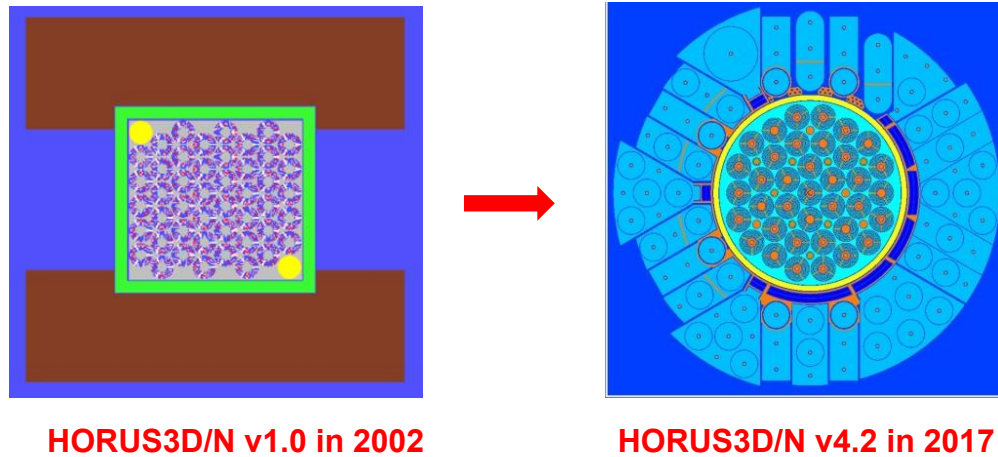
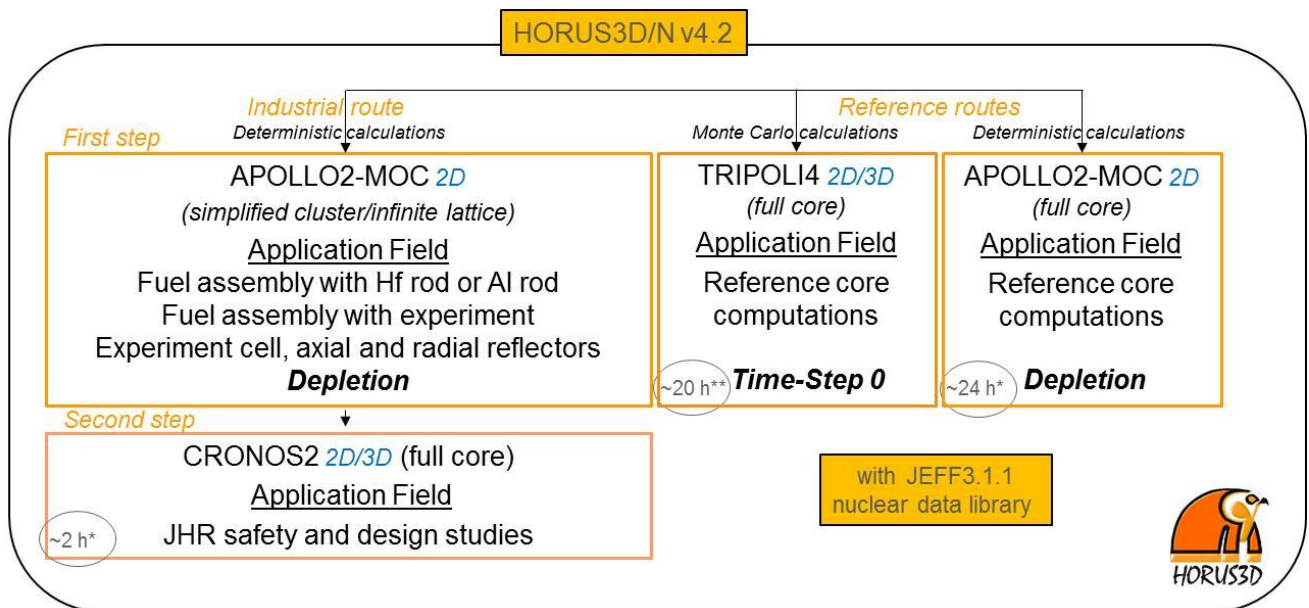


Fig.3. From HORUS3D/N v1.0 in 2002 to HORUS3D/N v4.2 in 2017



Calculations performed on an AMD Opteron Linux DELL 2.3 Ghz computer

* For full core computations, **depleted up to 82 GWj/t** (mean burn-up of the JHR core), on one processor

** For full core computations, **at time-step 0**, in parallel mode using 32 processors

Fig.4. HORUS3D/N v4.2 package calculation routes

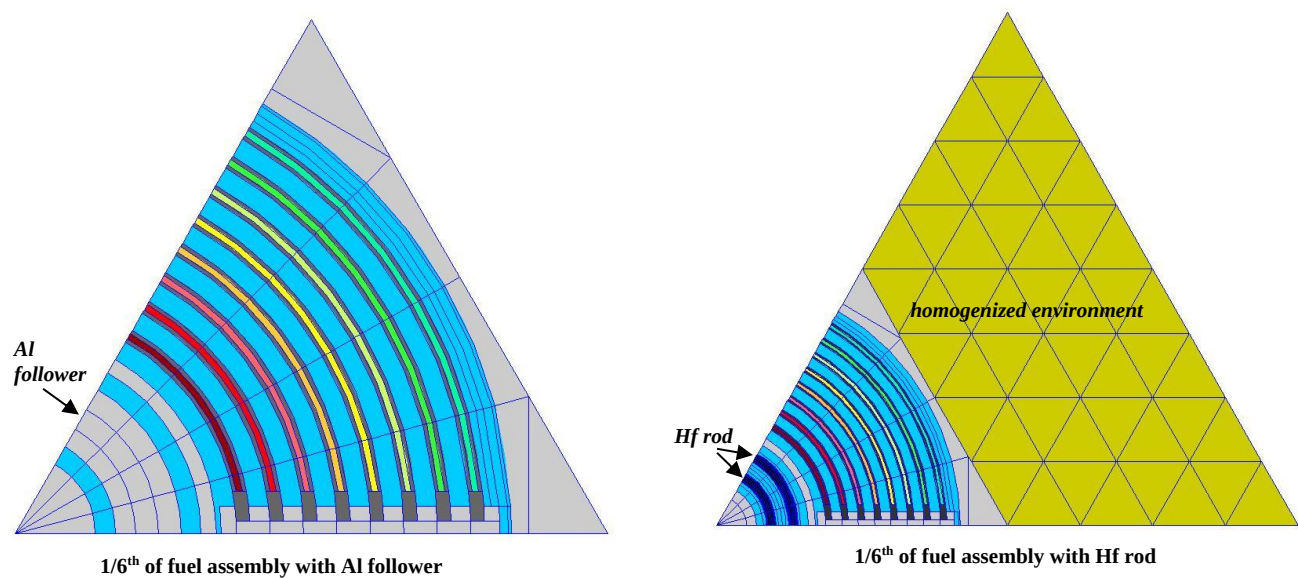


Fig.5. Flux computation geometry with APOLLO2-Method Of Characteristics flux solver

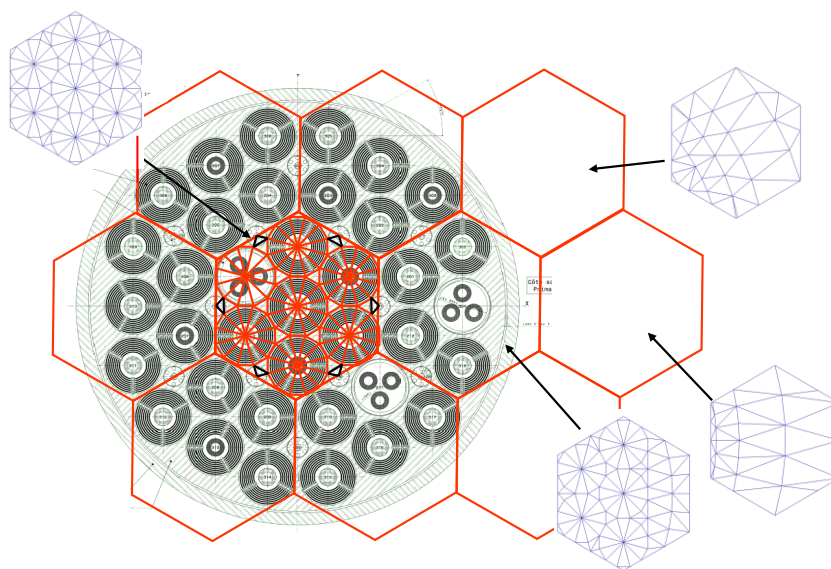


Fig.6. Hexagonal meshing (“Super Finite Element” - SFE) for CRONOS2 computations

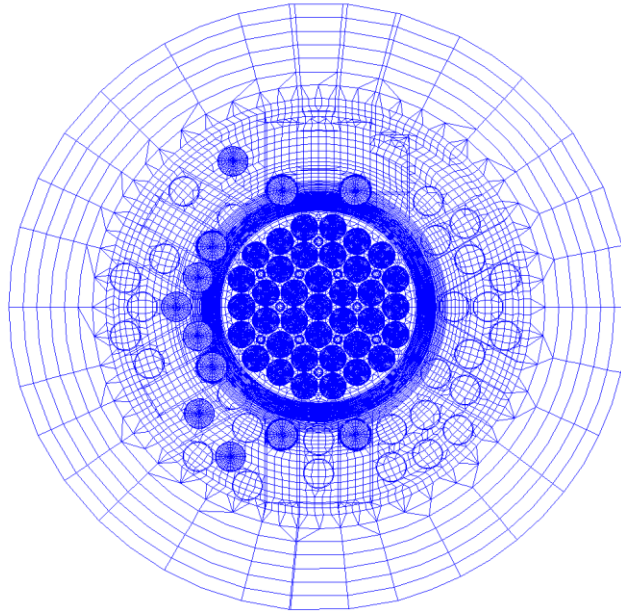


Fig.7. HORUS3D/N v4.2 core and reflector meshing

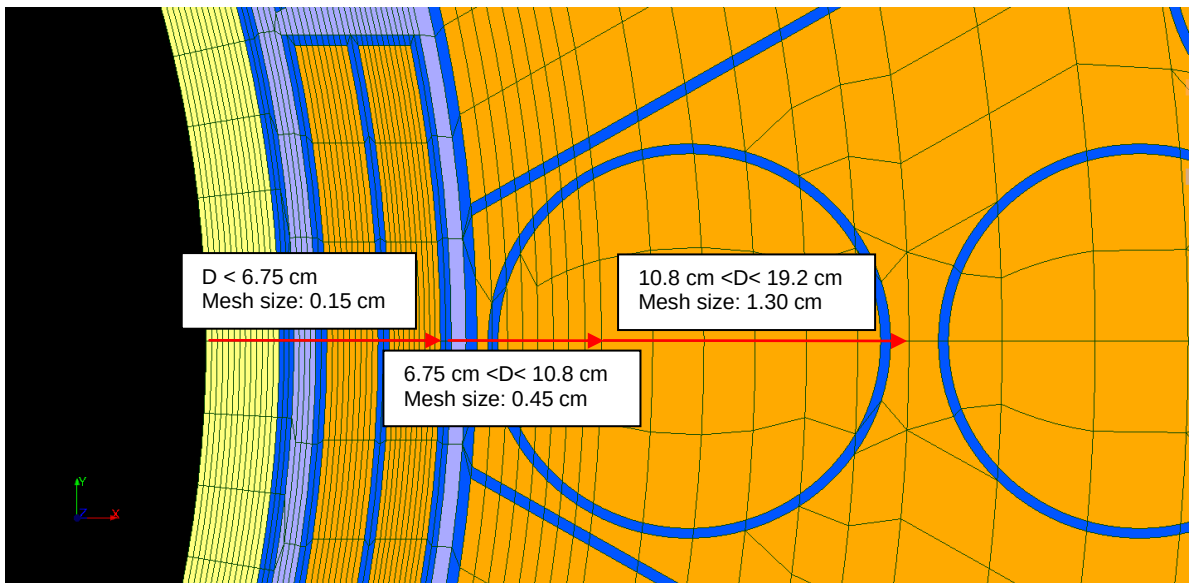


Fig.8. Reflector meshing with SALOME in compliance with APOLLO2.8/REL2005/CEA2005 package recommendations

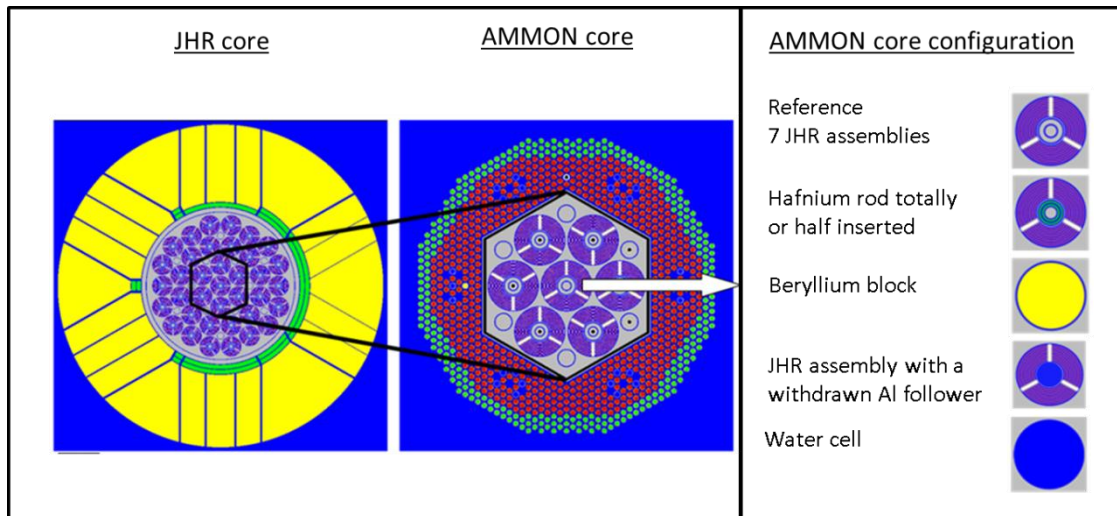


Fig.9. Configurations of the AMMON experiment

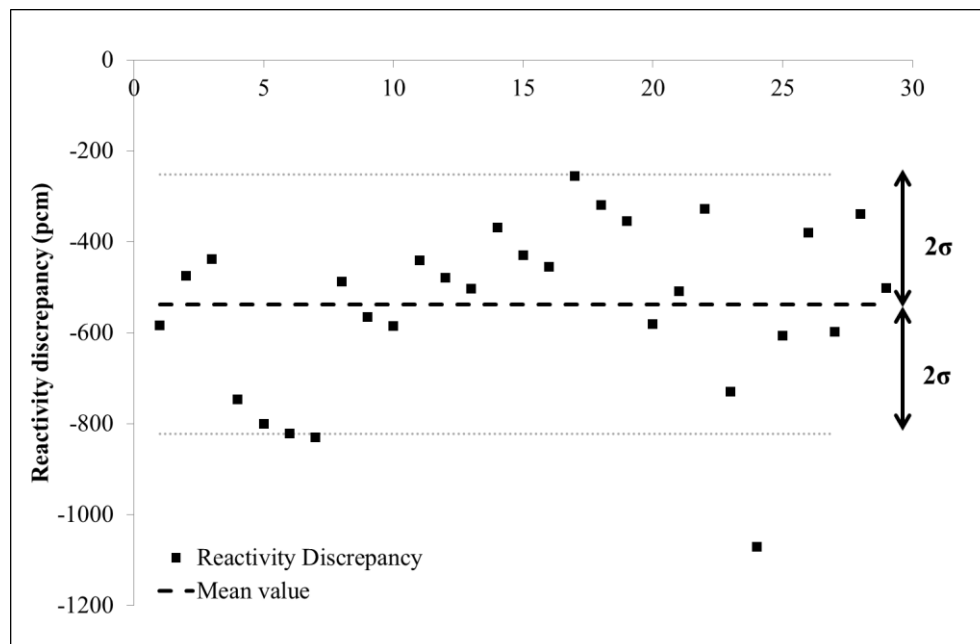


Fig.10. Scheme bias and uncertainty on reactivity calculation for rodded core configurations at step 0