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THE CRISTAL CRITICALITY PACKAGE: FROM 2.0 TOWARDS 2.1 VERSION

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ABSTRACT

The version 2 of the CRISTAL package, devoted to criticality safety calculations for safety enhancement and criticality risk prevention, was first released in 2014. Since then, four upgrades of its components led to the 2.0.3patch version. The development, verification and validation processes have been carried out in a joint project between the IRSN (Institut de Radioprotection et de Sûreté Nucléaire), the CEA/DES (Direction des EnergieS du Commissariat à l'Énergie Atomique et aux Énergies Alternatives), in collaboration with Orano group, EDF (Électricité de France) and Framatome. The CRISTAL V2.0.3 experimental validation database contains more than 3100 configurations representing the various configurations encountered in the fuel cycle. The CRISTAL2.0.3 package is available at the OECD Database.

In all its 2.0 versions, the CRISTAL package relies on the following extensively validated neutron transport codes and package key components: APOLLO2.8-3.C, MORET 5.B.1 and TRIPOLI-4.8. Each code uses the CEAV5.1.2 library based on the JEFF-3.1.1 nuclear data evaluation, for multigroup and continuous-energy calculations.
The link between the CRISTAL calculation codes is ensured by the LATEC workbench that allows users to generate all CRISTAL package input files, to launch calculations and to post-process outputs. The use of validated calculation options with the support of APOLLO2's dedicated procedures ensures high quality results and reproducibility.

The purpose of this paper is firstly to present the improvements brought by the latest 2.0.3 version.
Secondly, a presentation of the major upgrades of the future 2.1 version with a specific focus on experimental validation, new calculation tools, nuclear data libraries and functionalities, is made.

KEYWORDS

ICNC2023, Criticality safety, Calculation tools, CRISTAL package

1. INTRODUCTION

The CRISTAL V2 Project is a French collaborative project between IRSN (Institut de Radioprotection et de Sûreté Nucléaire), CEA (Commissariat à l'Énergie Atomique et aux Énergies Alternatives), Orano

and Framatome since 2008. It follows the CRISTAL V0 and V1 packages also developed and validated by IRSN, CEA, Orano, Framatome and EDF (Électricité de France) [1]. The first CRISTAL V2 package was released in 2014 with the V2.0(.0) version. The 2.0.1 version was issued in 2016 and the 2.0.2 in 2018. Both benefited from the industrial and safety organization users' feedback. The 2.0.2 [2] version was the first release distributed by the NEA (Nuclear Energy Agency) and the CRISTAL package was formally requested by more than 50 organizations across the world.
This article presents in a first part the latest 2.0.3 version [3], meant to be the last intermediate version of the CRISTALV2.0 and available since March 2021 for partners and September 2021 at the NEA Databank. The second part outlines the forthcoming 2.1 version expected by the end of 2024, including new versions of codes and optimized calculation sequences.

2. THE CRISTAL V2.0.3 PACKAGE

The CRISTAL criticality safety package provides four different calculation routes to address all calculations needs for criticality safety assessment, from standard calculations to 3D full modeling of a configuration. All these calculation routes use the cross-sections library CEAV5.1.2 based on the JEFF-3.1.1 evaluation. In the framework of the CRISTAL project, the calculation sequences of the deterministic code APOLLO2 were optimized on a criterion of computing time minimization while providing accurate results.
The development, verification, and validation processes of the CRISTAL V2.0.3 package [3] have been carried out in a joint project between the IRSN, the CEA, and in collaboration with French utilities Orano, Framatome and EDF.

2.1. CRISTAL V2.0 package architecture

The CRISTAL package is based on a modular architecture and relies on extensively validated neutron transport codes for criticality safety applications and useful tools.
The CRISTAL V2.0.3 package is detailed in [2] and consists of:

- the LATEC workbench in its 1.5 version [4],
- the nuclear data library CEAV5.1.2 based on the JEFF-3.1.1 evaluation [8], neutron transport codes, APOLLO2.8-3.C [5], MORET 5 [6] and TRIPOLI-4.8 [7].
- a set of specific calculation options for APOLLO2 code implemented in procedure libraries named APROC and APROC_CRISTAL.

These elements will be described in regard to their specific use in the CRISTAL package.

2.1.1 LATEC workbench

The LATEC workbench is a Computer Assisted Design user interface and the main entry-point of the CRISTAL Package. It is intended to be used on personal computer [4], driving the calculation code on a dedicated server or on a stand-alone installation on the user computer.
The criticality modeling software integrates a 3D geometry viewer and features to generate compositions of chemical mixtures of fissile nuclides based on dilution laws [9] and non-fissile media. LATEC allows switching easily between a homogenized multi-group calculation and a detailed pointwise one and can address all the CRISTAL package calculational routes.
LATEC also embeds a parametric and distributing computing engine to provide a consistent framework for criticality-safety studies. Hence, the user can provide various numerical values for different parameters. LATEC will then automatically generates the input files and perform the calculations related to these values.
LATEC is designed to allow both skilled users and beginners to achieve consistent and reliable studies in an industrial context. A quality assurance approach in the modeling process is included to support the whole life cycle of a study as LATEC can hold the full criticality-safety study workflow, including parametric calculations, model verification and versioning.

2.1.2 Nuclear data files

All the neutron transport codes within the CRISTAL package use the same nuclear data library CEAV5.1.2, processed by the GALILÉE tool [10] and based on the European JEFF-3.1.1 evaluation [8]. This process produces consistent continuous-energy and 281-energy groups data, respectively for the reference continuous-energy Monte Carlo code TRIPOLI-4® [7] and for the multigroup-energy APOLLO2 [5] and MORET 5 [6] transport codes.
For APOLLO2 and MORET 5, the standard multigroup CEAV5.1.2 library is available for various temperatures beyond 273 K and an additional specific library provides the required data for 18 nuclides at 214 K.
For TRIPOLI-4®, the standard CEAV5.1.2 pointwise library also includes probability tables that are calculated on a 11513-energy grid for an energy ranging from 10^{-5} eV to 20 MeV, shared with APOLLO2. The available temperatures are 214 K (for the 18 nuclides mentioned above), 294 K and 300 K.

2.1.3 APOLLO2 Code

The APOLLO2.8-3.C version, available within the CRISTAL package is a version of APOLLO2 code dedicated to criticality calculation. APOLLO2 [5] is a neutron transport code developed by CEA based on deterministic methods.
In the CRISTAL package, the APOLLO2 code generates the cross-sections file, using the collision probabilities method, that will be used by APOLLO2 (Sn solver) or MORET 5 Monte-Carlo code to provide the effective multiplication factor. Spatial homogenization as well as energy collapsing, if necessary, can also be done on the self shielded cross-sections.
The APOLLO2 Sn neutron-flux solver is also used for criticality standard calculations to determine reference values. Indeed, an algorithm is available to perform iterative Sn calculations in order to find the dimension of simple standard 1D geometries for a user defined k_{eff} value. The validation of the APOLLO2 code relies on comparisons both to Monte Carlo calculations and experimental measurements coming from numerous experimental programs.

2.1.4 MORET 5 Code

The MORET 5 code [6], developed by IRSN, solves the transport equation for neutrons using the Monte Carlo method. It is used to support criticality safety assessments and was developed to match the needs for nuclear fuel cycle facilities and fissile material transport. The MORET code allows users to model three-dimensional geometrical configurations based on combinatorial representation with predefined shapes and operators. MORET 5 can use continuous and multi-groups data for criticality calculations. However, only the multi-group release is available in the CRISTAL package. Version 5.B.1 of the MORET code applies only to the multi-group route with APOLLO2 homogenized cross-sections. It uses multi-group cross-sections from the APOLLO2 cell code to describe the materials and the user can select, from all available methods, the most appropriate simulation method related to its problem, define tallies and analyse the results.

2.1.5 TRIPOLI-4® Code

TRIPOLI-4® [7], developed by CEA, solves the linear Boltzmann equation for neutrons with the Monte Carlo method, in any 3D geometry. TRIPOLI-4® has its own native geometry package, allowing for both a pure surface-based representation, and a combinatorial representation with predefined shapes and Boolean operators (any combination of these two kinds of representations can be adopted).
Within the CRISTAL package, TRIPOLI-4® uses the standard nuclear data library, CEAV5.1.2 which is mainly based on the European evaluation JEFF-3.1.1. The probability tables used by TRIPOLI-4® in the unresolved resonance range are generated using the CALENDF [12] code and are given in separate files. CALENDF first converts resolved and unresolved resonance parameters into temperature-

dependent continuous-energy cross-sections. Then, relying on Gauss quadrature principle, the code generates "cross-section probability tables" (PT) on a user-specified energy grid. TRIPOLI-4® uses these tables in the unresolved resonance range for each nucleus and during the Monte Carlo transport simulation the PT supersede the continuous-energy cross-sections available in the original PENDF files. The 8.1 version of TRIPOLI-4® is included in CRISTAL V2.0.3.

2.2. Calculation routes

2.2.1 Multi-group Routes

These routes are based on two main steps. In the first one, shared by both M.D. (Multigroup Deterministic) and M.MC (Multigroup Monte Carlo) routes, the APOLLO2 code generates multi-group self-shielded cross-sections for each medium or lattice cell that will be used in the studied configuration. The APOLLO2-MORET 5 route is used in more than 90% of criticality safety studies. The APOLLO2 calculation gives physically representative cross-section sets, with an accurate description of reaction rates in the real geometry. In a first step the Pij (Collision Probability Method) neutron flux solver is used for the flux calculation, which can be used for a spatial homogenization of the self-shielded cross-sections sets.
In a second step, those homogenized self-shielded cross-sections are used by the MORET 5 multi-group (281 energy groups) or by the Sn solver of APOLLO2 (in CRISTAL scheme, collapsed on 20 energy groups) in order to evaluate the effective multiplication factor of the system and its associated standard deviation for the Monte Carlo route. In this context, all the elementary volumes are assumed to be homogeneous and are described, at the collision level, by an equivalent nucleus. Regarding the MORET 5 calculations, the spatial distribution of the sources for the first cycle can be described in any of the following ways: automatically throughout the entire system, volume by volume, or as individual points. To estimate the bias due to the use of a deterministic code, the user can convert automatically with LATEC workbench its input file into TRIPOLI-4® one.

2.2.2 Point-wise Monte Carlo Route (P.W.M.C.)

The point-wise Monte Carlo route (P.W.M.C. Route) relies on the TRIPOLI-4® Version 8.1 associates with the CEAV5.1.2 pointwise library the use of probability tables at 294K. It can be used for reference calculation or for industrial calculations when needed. Used in its "criticality mode", the Monte Carlo code TRIPOLI-4® is used to solve the k_{eff} eigenvalue equation. An initial neutron source guess is set for the first batch, and the equilibrium neutron distribution corresponding to the k_{eff} eigenvalue equation is then sought. For this purpose, the power iteration scheme is adopted: at the end of each batch the secondary neutrons generated from fissions are used as a source for the next batch. Between batches, a normalization procedure is applied, as customary. After several steps, when the distribution of fissions has converged, the neutron distribution obeys the fundamental mode of the keff eigenvalue equation. Then, the physical quantities of interest can be scored. The convergence criterion can be either defined by the user, or automatically set by the code by resorting to statistical tests so as to assess whether equilibrium has been reached.

2.2.3 Criticality Standard Calculation Route

In addition to the three calculation routes previously introduced, a specific route is provided for criticality standard calculations. One spatial dimension configurations including several combinations of media (fissile material and reflectors) can be modeled. The dimensions of each material corresponding to a target k_{eff} is determined with a given precision by an iterative process.
A specific module, dedicated to the numerical embedded inaccuracies of the Sn method, is available and allows the user to obtain amended values. It allows to quantify the intrinsic Sn calculation biases during the iterative calculations. The estimated k_{eff} is then corrected by the given calculation biases in order to provide a new dimension value corresponding to a target k_{eff}. During the iterative calculation process,

the calculation biases are quantified by direct calculations comparisons (for the energetic mesh and for the anisotropy order - depending on the available data) or by the use of the KATO formula (for the spatial mesh and Sn order - to simulate the use of infinite values).
However, the interaction between fissile and reflector media is not taken into account for the macroscopic cross-sections generation, which can lead to inaccuracies when calculating some heterogeneous configurations. To estimate this effect, a continuous-energy calculation can be done using TRIPOLI-4®, in order to check the corrected deterministic calculation results. Thus, the LATEC workbench can automatically generate the TRIPOLI-4® data file corresponding to the APOLLO2 result allowing the user to estimate the APOLLO2 Sn bias.

2.3. CRISTAL package validation

The CRISTAL V2.0 package benefits from a broad experimental validation database covering almost all areas of criticality-safety applications. 3,127 critical experiments, corresponding to 342 series, either issued from the OECD/ICSBEP Handbook [13] or performed in French facilities (confidential data) were selected for the CRISTAL V2.0 validation database. Currently, nearly 2,400 experiments are modeled, analysed and part of the validation database [14]. The validation database will continuously be expanded to reach the aimed number of selected experiences. Some of these experiments are modeled with the three CRISTAL routes (APOLLO2-Sn, APOLLO2-MORET 5 and TRIPOLI-4®).

2.3.1 Validation database and associated process

A dedicated technical working group within the CRISTAL Project selected a set of experiments according to the demands of both users and code development entities in order to define the CRISTAL experimental validation database. Main sources are the OECD/ICSBEP [13] and additional experiences performed by IRSN and CEA with the financial support of industrial. This work consisted in choosing a sufficient set of experiments from various laboratories in order to avoid bias due to correlations between experiments and to avoid systematic errors in the experiments.
The validation process is a standard one and consists in calculating the C-E value using recommended calculation sequences of the CRISTAL package. All C-E values are given by calculated k_{eff} minus benchmarks k_{eff}, and its combined one standard deviation.
The comparisons with other available experimental programs in the same field (similar media, materials and/or configurations) allow for highlighting potential experimental biases.
In a second step, (C - E) discrepancies are analyzed in order to uncouple the different causes of calculation biases and so, get feedback on the nuclear data and/or to the calculation sequences. The consistent evaluation process for the nuclear data libraries generation within the CRISTAL package allows inter-code comparisons between the different CRISTAL V2 routes. Furthermore, in a R&D process, inter code comparisons are also done by using other cross-section libraries (as ENDF-B/VII.0) with the TRIPOLI-4® continuous-energy code. The use of other available calculation results from international codes (MCNP, SCALE, MONK, etc…) using various nuclear data libraries is also in this R&D process. In addition, CRISTAL package results are available in some ICSBEP benchmarks proposed or reviewed by IRSN.
Eventually, an open validation document gathering many ICSBEP benchmark results, and their analysis will be available with open access. This document will be released in 2023 for the CRISTALV2.0.3 version.

2.3.2 Main results

Calculation results obtained on the whole set of modeled experiences shows a general good agreement with the benchmark k_{eff}. The CRISTAL package is validated for a wide range of criticality safety application. Some discrepancies were observed for the following cases:

- slight overestimation for plutonium solutions,

- small underestimations or overestimations for arrays of fuel pins depending on the moderator to fuel ratio,
- underestimation for fuel rods array including holes (case of missing rods in fuel assemblies) due to the M.M.C. routes,
- overestimation for MIX-MISC-THERM series without poison,
- significant over-estimations with the multi-group calculations routes for reflected configurations with thick structural materials mainly in fast spectra.

3. THE FUTURE 2.1 VERSION OF THE CRISTAL PACKAGE

The 2.0.3 intermediate version is the last of the CRISTAL V2.0 package. A wide consultation amongst the partners was done to identify needs of new features, calculation sequences upgrades and improvements to the user experience in order to keep the package up-to-date and able to answer to any new issue within the criticality safety assessment field.
This work was achieved by the end of 2021, and it was concluded that although the majority of the improvements concern the LATEC GUI, some of the major desired features includes the integration of new versions of the neutron transport codes combined with enhanced calculation sequences of APOLLO2 code. Thus, from calculation sequences to neutronic codes including validation process and new tools, the CRISTAL V2.1 will be fully renewed to keep its functionalities up to date.
The following sections highlight these main changes.

3.1. Nuclear data

In the future version of CRISTAL package, the nuclear data will still be based on the JEFF3.1.1 evaluation [8] but with renewed probability tables and a more precise energy grid going from 281 to 383 groups [15]. Probability tables outside unresolved resonances domain have been regenerated for the deterministic code with the GTREND [16] module of GALILEE-1 [10], the new validation and processing system for evaluated data, developed at CEA. For the release later than CRISTAL V2.1.0, users would be able to use nuclear data based on other evaluation, such as ENDF-B/VIII.

3.2. Transport codes

3.2.1 APOLLO2 code

The deterministic code APOLLO will be at the 2.8-5.C version, a specific version created from the APOLLO2.8-5.PATCH2 without depletion calculations. The major novelties for the CRISTAL package in the code, are new functionalities such as XML output coherent with the TRIPOLI-4® XML output (same XML tags ensuring easiest comparison via post treatment) and some restriction on self shielding computations that are suppressed ensuring a better treatment for the CRISTAL package.

3.2.1 MORET code

The MORET 6 code [16] will replace the MORET 5 code. Initially designed for criticality calculation, the new features enhance the MORET code criticality capabilities with the multigroup sensitivity coefficient to nuclear data calculation, the new fission matrix calculation algorithm and the possibility to simulate randomized geometry. Furthermore, a volume calculation and a complete rewriting of the volume selection mechanism within the code are part of the modifications brought by the MORET 6 version. The MORET 6 code will also be helpful for applications relevant for safety as it shows good agreement with experimental value on neutron noise benchmarks and the possibility to use analog fixed source simulation for dedicated calculations. However, these functionalities are not available for pure criticality safety studies. Finally, multiple features have been added in order to improve the use of MORET code by facilitating the creation and checking of input data. A specific version of the MORET 6 code, dedicated to criticality calculations, will be integrated in the CRISTAL package.

3.2.1 TRIPOLI-4® code

The 4.12 version of TRIPOLI-4® will constitute the reference continuous-energy Monte Carlo code of the package, with a specific version 4.12-C dedicated to CRISTAL, without depletion calculations. A lot of new features are available since version 4.8 of the code. More than thirty improvements and new features related to criticality neutron transport and tallies have been implemented [17], such as the use of MORET geometries, a generator of stochastic geometries, super-history and Wielandt methods for direct and adjoint criticality calculations, various perturbations and sensitivities capabilities (standard and generalized perturbation theories), stochastic temperature interpolation for cross-sections and probability tables Diven factor, kinetics parameters, fission matrix on a mesh and Doppler Broadening Rejection Correction of the elastic cross-section. The use of MORET native geometry package was requested by user to facilitate the conversion of complex geometry modelled with MORET into TRIPOLI4 input file.

3.3. Calculation sequences

The calculation sequences will be upgraded in order to take into account the precision gained by increasing the number of groups in the grid. Self-shielding procedures will also be upgraded, with the use of the subgroup method. All calculation options will also be reviewed in order to offer optimized calculation sequences.

3.4. LATEC

The LATEC workbench, that will be in its 2.0 version, will integrate ergonomic improvement of the GUI, such as material panel, archiving capabilities, and bug fixes. More than 200 improvements or modifications are planned to be included in the new version. Aside its visual upgrade, and a new 3D viewer, the LATEC, will not only take into account the new codes and the new calculation sequences but will also provide new functionalities permitted by the new codes. The implementation of randomized geometries for MORET and TRIPOLI-4® will be available to the user in the LATEC workbench. A complete rewriting of the dilution law is also underway, and these laws will be available outside the bench via Python interface. Sensitivity studies will also be natively assessed by the GUI and will allow to provide data for the CRESUS software (see 3.5). New algorithms will also be integrated and available for the users to enhance criticality safety calculation studies.

3.5. Validation

As the package development is still underway, the validation process has not started but preliminary R&D results show better agreement with the reference calculation and experimental k_{eff} on some cases that were problematic with the previous version of the package. The full package validation process is scheduled to begin mid-2024. Nevertheless, two novelties are scheduled and can be assessed in this article.

First, in order to help the user exploit the validation database, a dedicated software will be released at the same time: CRESUS (Cristal Results & Estimation of Sensitivity and Uncertainty Software). Its purpose will be in a first step to help the user selecting experimental cases in the database that correspond to its application case. From this, it will be possible to know the confidence in the results regarding the validation cases in the CRISTAL package database. More functionalities will be implemented in further versions of the tool.

Furthermore, the open validation document gathering many ICSBEP benchmark results and their analysis will be available with open access and will focus specifically on the 2.1 version.

The validation database will also be extended towards the less considered types of experiences in the current database.

4. CONCLUSIONS

The CRISTAL V2.0.3 package represents a consistent and powerful integrated system combining well validated calculation codes and sequences. The LATEC workbench proposes a high level of user-friendliness, flexibility and quality assurance. The validation work pointed out that the calculation results are generally in good agreement with the benchmark k_{eff}, which ensures to the CRISTAL package optimal performance for criticality-safety calculations. It is also available for both partners and international users since 2021. This version is meant to be the last of the CRISTAL V.2.0 versions, so a wide consultation amongst partners led to the conclusion that new functionalities were needed implying the integration of up-to-date calculation codes and new tools developments.
The future CRISTALV2.1 version will thus not only integrate the feedback of the latest CRISTALV2.0.3 version but will also benefit from the integration of the latest versions of its main components (nuclear data libraries, transport codes and calculation sequences).
A specific item on internationalization of the package with English error messages and input data descriptions put together with an open validation document will support the release of the version in an effort to widen its use.
CRISTALV2.1 is meant to be released by the end of 2024, first for partners involved in the development of the package and later to the international community.

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