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High Resolution Modelling without Computation Slowdown for PETALE in CROCUS

T. Ligonnet¹, A. Laureau^{2,3}, V. Lamirand^{1,4}, and A. Pautz^{1,4}

¹Laboratory for Reactor Physics and Systems behaviour (LRS),
Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

²SUBATECH, CNRS/IN2P3
IMT-Atlantique, F-44307 Nantes, France

³Univ. Grenoble Alpes, CNRS,
Grenoble INP, LPSC-IN2P3, 38000 Grenoble, France

⁴Nuclear Energy and Safety Research Division (NES),
Paul Scherrer Institut (PSI), CH-5232 Villigen, Switzerland

thomas.ligonnet@epfl.ch, axel.laureau@subatech.in2p3.fr, vincent.lamirand@epfl.ch,
andreas.pautz@epfl.ch

ABSTRACT

The PETALE experimental program was successfully carried out in the CROCUS reactor of EPFL in the fall of 2020, in a collaboration between EPFL and CEA. It consists of criticality and transmission experiments with four distinct metallic reflectors made of 304L stainless steel, iron, nickel, and chromium, to study the nuclear data of stainless steel. In addition to the experimental results, one of its outcomes is the production of C/E and their covariance matrices for the reaction rates of the dosimeters used in the transmission experiments, with the aim of allowing to constrain future nuclear data evaluations. For this purpose, the chosen methodology for uncertainty propagation is the computationally expensive Total Monte-Carlo method. A modified build of the Serpent2 Monte Carlo transport code is used to perform Variance Reduction and correlated sampling. In addition, high resolution modelling of the experiments is used to limit the presence of bias in the analysis, and to pave the way toward the submission of a high-quality benchmark to an NEA database. This paper presents advances in the modelling of the experiments, focusing on the metal reflectors, as installed at the periphery of CROCUS. It was possible to refine from a simple design model made of a few cuboids, to a fully detailed model, while keeping the loss in computational efficiency below 15%. Notably, all reflector sheets of PETALE were detailed into 121 voxels each, based on topological measurements, without impact on the calculation time, thanks to the use of Serpent2 3D lattices.

KEYWORDS: Monte Carlo, Modelling, Voxelization, Integral Experiments, Iron Nuclear Data, CROCUS.

1. INTRODUCTION

The EPFL-CEA PETALE (*Programme d'Étude en Transmission de l'Acier Lourd et ses Éléments*) experimental program [1] is dedicated to the study of nuclear data of stainless steel and its main elements, iron, nickel, and chromium. It was successfully carried out in fall 2020 in the EPFL light water zero power research reactor CROCUS. The first output of the program is the measurements of reaction rates for selected dosimetry reactions as a function of penetration depth in the metallic reflectors, i.e., transmission experiments. A second output is the production of C/E (computation-experiment ratio) for the aforementioned reaction rates through Monte-Carlo simulations, using state of the art nuclear data libraries for the neutron transport, and the specialized library IRDFF for the dosimetry reactions [2].

Integral experiments have the advantage of allowing low experimental uncertainty and, with appropriate covariance evaluations, are useful in validation [3] and evaluation [4] processes, and needs were identified for the case of iron [5]. From the inception of PETALE, the aim was to produce results of use for the nuclear data community, by ensuring that the results are constraining the nuclear data. In this aim, in the design phase, target experimental uncertainties were quantified thanks to the propagation of nuclear data uncertainties in a preliminary experimental setup and its corresponding *design model* [1,6], by using Total Monte Carlo (TMC). In the on-going analysis phase, the same uncertainty propagation approach is consistently chosen [7] to produce a detailed uncertainty budget with covariances. It requires a *refined model* of the experiments that reproduces PETALE extensively: the purpose is to limit as much as possible biases arising from geometries and materials in the C/E, and to quantify the impact of their uncertainties. Thus, it includes the definition of material cards through chemical analysis for an extensive number of alloys, and sometimes even multiple definitions for different production batches. In addition, it includes all structural parts, and the metallic reflector sheets are voxelated following micrometric topological measurements.

Five different modelling approaches are tested for modelling the same and single experimental setup corresponding to the iron reflector case. The models range from the raw *design model* to a complete *refined model* of PETALE making extensive use of Serpent universes and lattices, passing through the two approaches tested to accurately voxelate each of the eight reflector sheets: *cuboidal* and *lattice*. The additional *cuboidal_FT* model allows to study the impact of transformations. The need for each part to be able to move freely with respect to their free space is kept in mind for all models, in order to allow the estimation of positional uncertainties through Monte-Carlo simulations of randomly perturbed geometries. A profiling was performed for each model to assess function loads and sources of slowdown. Finally, the computational characteristics and performances of all models are compared.

2. SIMULATIONS

2.1. Software and Variance Reduction for PETALE

Simulations for the analysis of PETALE are performed using a modified build of Serpent 2.1.21 [8]. This build, developed in-house in preparation of PETALE, and updated for the work at hand, contains a Variance Reduction method to accelerate the convergence of PETALE dosimeters [6].

A weight map is produced and updated along the simulation, on a distance-to-hit basis, to allow a one-step calculation. In addition, this build allows to perform correlated sampling (CS), a functionality that will be used to perform Bayesian Monte-Carlo Assimilation with PETALE results [7,9]. The drawback of these additions is the inability to use delta-tracking, as it is incompatible with the implementations.

2.2. PETALE geometry and modelling

All four reflectors of PETALE consist of the same aluminum case that contains eight 2-cm thick metallic sheets of about 30×30 cm of the studied material, and nine dosimeter holders set before, in-between, and after them (see Figure 1). Each dosimeter holder carries up to nine cylindrical activation dosimeters, with a diameter of 29.5 mm and a thickness of about 0.5 mm (except for gold dosimeters: 0.01 mm). In addition, the reflector case is surrounded by structural parts that allow its accurate positioning in the periphery of CROCUS, at short distance from the core, on the order of 5 mm to the next fuel rods depending on the reflector material and corresponding weight. In this study, the iron reflector is used as a test case.

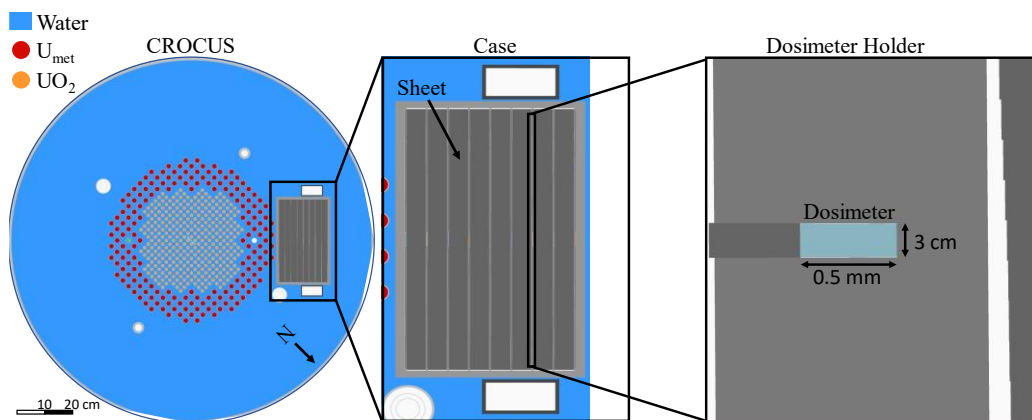


Figure 1. Axial cross section of the PETALE configuration: starting from the CROCUS vessel (left) to close-ups on first the case and its metal sheets (middle), then dosimeter in a dosimeter holder (right). In the latter close-up, the voxelization of a neighboring reflector sheet is visible on the right.

The objective of the modelling is not only to compute the dosimeters' reaction rates, but to propagate the geometrical uncertainties to the reaction rates. For this purpose, a sampling approach is used. A python script was developed to automatically produce each of the 26 PETALE experimental geometries with the option to randomly perturb the geometries' parts positions. The case itself is moved according to the uncertainty on each of the measurements defining its position in the reactor, and each element in the case is moved with respect to their mechanical clearance. Thus, each part is defined to allow group and individual motions.

2.2.1 Models for reflector voxelization

The first step of the model refinement, from the raw *design model*, is the voxelization of each of the reflectors' metallic sheets. Using the data obtained through topological measurements regularly done on each face, each sheet is voxelated into 121 voxels. The plots in Figure 2 display an example of topological measurement outputs. Two approaches guaranteeing the same refinement level are tested.

The first approach, named here *cuboidal*, is a conventional and direct use of Serpent cuboid surfaces to define each voxel of a sheet and to fill them with the reflector material, thus creating 121 cells. Then a larger cuboid enveloping all the voxels is defined in order to fill the remaining space with air in a 122nd cell.

The second approach, named *lattice*, takes advantage of the regularity of the topological measurements. In this case the reflector' sheets are defined using $11 \times 11 \times 1$ Serpent2 3D lattices, each sub-universe of a lattice being a voxel. In this case, each voxel volume is identical and contains both air and metal separated by surfaces. For this model three type of voxel are differentiated, those at the center (81 voxels), the sides (36 voxels), and the edges (4 voxels) of the sheet. At the center, the voxels are defined by two surfaces delimiting the upper and lower boundaries of the sheet, the sides being defined by the lattice X and Y pitches. On the sides a third surface is necessary to reflect the topology of the sheet's smaller sides, as well as a fourth surface in the case of edges.

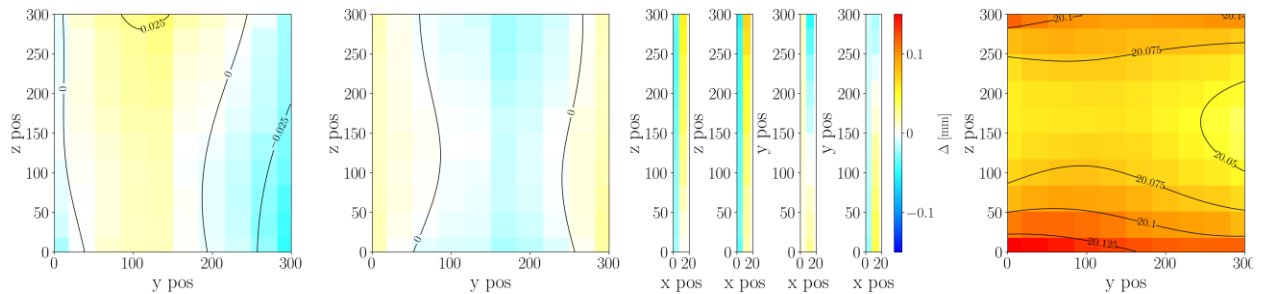


Figure 2. Example of topological measurements for a sheet, in this case a chromium one. The first two pictures are the topological measurements of the front face and back face of the sheet. At the center are the four sides of the sheet. On the right image is displayed the local thickness of the sheet.

2.2.2 Refined model and structure optimization for computation acceleration

The *refined model* includes the addition of all structural parts and all compositions, in addition to the voxelization of metallic sheets using the *lattice* approach. The geometry of PETALE encourages the use of cells directly defined using neighboring cuboid surface to easily model the geometries, as most of its internal and structural parts are cuboidal, and either separated by air or water. Nevertheless, the multiplication of cells and surfaces is required to accurately reproduce the geometry and the isotopic composition of all pieces. It was hypothesized that the code slows down

because of the number of operations that it performs to assess in which cell a neutron is, rather than the number of parts in the geometry itself. As a particular interest is given to the fidelity of the geometry, rather than simplifying the model, the solution finally chosen is to rework the geometry entirely in order to take advantage of the definitions of Serpent universes and nested universes. As a consequence of the model refinement, the geometry of the case evolved from a single level geometry containing a single universe and a total of 70 cells for the design model, to a complete *refined model* of PETALE on 4 levels with 975 universes, including the lattices sub-universes, and a total of 3407 cells.

2.3 Models profiling and test model *cuboidal_FT*

Profiling of the different models are performed to assess if any functions are especially time consuming for a given model and how it is connected to the geometry definition. The profiling was performed with the GNU profiler *gprof* included in the GNU Binutils 2.39 release[10]. The percentage of time the code is passing in a function is used as an indicator to compare the different models. The profiling allows to observe which functions are the most heavily relied on depending on the geometry definition. However, it does not give direct and quantitative information on the code running speed, as the profiling itself is substantially affecting it. One qualitative indicator is the percentage of time the code is passing in the “MoveST” function and its sub-called functions as it is in competition with functions that can, in most cases, be considered independent of the method used to define the geometry. The relative FOM is used to quantitatively compare the different model convergence speed.

The profiling of the *cuboidal model* shows that, during the simulation, the code is spending 91.87% of the time in the function “MoveST”. Most of this time is actually passed in sub-called functions, the intrinsic time percentage of the “MoveST” function being only 0.09%. The noticeable contributors with their intrinsic time consumption are: “CoordTrans” with 67.6%, “TestSurface” 7.55%, and “SurfaceDistance” 10.7%. The function handling coordinate transformations, such as rotation and translation, is commonly called by the two other and is the most expensive function in total computation time. The reason is that during the definition of PETALE, each of its surfaces are declared around the geometry origin. Then, each of them is independently translated to the real experimental position.

From this result, a new model *cuboidal_FT* was created. In this model all PETALE surfaces are declared in a sub-universe to factorize all surface transformations in a single universe one. The profiling shows that in this case the percentage of time passed in the function “MoveST” is decreased by 12 % to 79.29%, with an intrinsic contribution of 0.22%. The contribution of “CoordTrans” is significantly decreased to 3.46%, but this decrease is partly compensated by the increase in the percentage of other function, some of which have negligible intrinsic time consumption in the simple *cuboidal model*: “TestSurface” 16.36%, “SurfaceDistance” 28.72%, “InCell” 18.58%, and “NearestBoundary” 8.89%. Those increases are mostly due to the renormalization of the percentages following the decrease of the time spent in “CoordTrans”, but it is noticeable that the time consumption of the function “InCell” has a larger increased than other functions. It can be explained by the fact that “InCell” is called by the “FindUniverse” function, which has seen its usage increased by the newly added universe in the geometry definition. As presented in next part and in Table 2, the model FOM has significantly increased following the

factorization with respect to the *cuboidal model*, but it is still inferior to the results obtained with the following *lattice model*.

For the *lattice model*, the time the code is spending in “MoveST” is significantly reduced with respect to the two *cuboidal models*, the total time percentage is 41.17%, with an intrinsic contribution 0.5 %. In this case the intrinsic time consumption of all previously mentioned function has decreased with respect to the *cuboidal_FT* model. The only exception being the “CoordTrans” function because which increased due to the percentage renormalization. On the other hand, a new function “FindLatticeRegion” is now used but with a low 1.1% of time consumption. In particular, the time the code is taking to find the distance to the nearest surface, and in which cell the particle is, has sharply decrease. The relative time consumption of each function of interest and model is presented in Table 1.

Table 1. Relative time consumption for function of interest for each model. The upper percentage is the intrinsic time consumption, the lower percentage (in parenthesis) is the total time consumption, including sub-called functions.

Function \ Models	<i>Design</i>	<i>Cuboidal</i>	<i>Cuboidal_FT</i>	<i>Lattice</i>
MoveST	0.50 % (50.18 %)	0.09 % (91.87 %)	0.22 % (79.29 %)	0.53 % (41.17 %)
CoordTrans	12.86 % (12.86 %)	67.59 % (67.59 %)	3.46 % (3.46 %)	8.65 % (8.65 %)
NearestBoundary	2.72 % (12.75 %)	1.66 % (31.98 %)	8.89 % (38.79 %)	3.10 % (9.50 %)
SurfaceDistance	5.27 % (10.02 %)	10.70 % (30.32 %)	28.72 % (29.90 %)	3.43 % (6.40 %)
InCell	17.76 % (29.12 %)	3.94 % (59.34 %)	18.58 % (36.39 %)	13.12 % (21.16 %)
TestSurface	3.28 % (11.35 %)	7.57 % (55.41 %)	16.36 % (17.81 %)	2.82 % (8.04 %)
FindLatticeRegion	<0.5%	<0.5%	<0.5%	0.91 % (1.11 %)

2.4 Models performances

The simulation results show that the voxelization of the reflector sheets does not increase in computation as the model mean relative FOM stays at 1. Conversely, if the reflector is voxelated using cuboid surfaces, the total computational time is multiplied by a factor 4.3. This result shows the main advantage of this lattice approach: it allows to significantly increase the accuracy of the geometry with respect to the experimental setup, while only moderately complexifying it, and to keep its computational efficiency.

Following the profiling and the study of the additional *cuboidal_FT model* with a factorized transformation of the case universe, the factorization significantly reduces the computation time by a factor 2.5. The reason individual surface transformations were originally preferred is that it makes it simpler to perturb the geometry. Indeed, in the *cuboidal model* the perturbations are simply added to the surface transformation, while in the *cuboidal_FT model* it is necessary to modify the surface cards themselves, making it more ambiguous and prone to errors.

Following these changes in definitions, the *refined model* and its computational efficiency loss was limited to a +15% increase with respect to the *design model*, as visible in Table 2 with the relative Figure Of Merit (FOM)[6]. Following the benefits of lattices and universes on calculation time, the decrease in calculation efficiency with the *refined model* is believed to be caused mainly by the increase in thermal neutrons streaming in the additional structural parts, rather than by the increase in cells number.

Table 2. Characteristics of the simulations and relative Figure Of Merit (FOM) for the three models, with respect to the design model of PETALE.

Models \ Characteristics	<i>Design</i>	<i>Cuboidal</i>	<i>Cuboidal_FT</i>	<i>Lattice</i>	<i>Refined</i>
Histories (10^6)	577	82	210	592	684
CPU Time (h)	313.75	335.27	310.73	323.40	333.73
RAM (GB)	8.2	8.2	8.2	8.2	8.2
Mean Relative FOM	1	0.23	0.59	1.01	0.87

The simulation results obtained for the 10 $^{197}\text{Au}(n, g)$ dosimeters, placed in the case, for the *lattice model* and the *cuboidal model* are consistent. Indeed, all computed reaction rates for the *lattice model* are at less than two standard deviations from their counterpart of the *cuboidal model*, with seven out of ten at less than a standard deviation, as displayed in Figure 3.

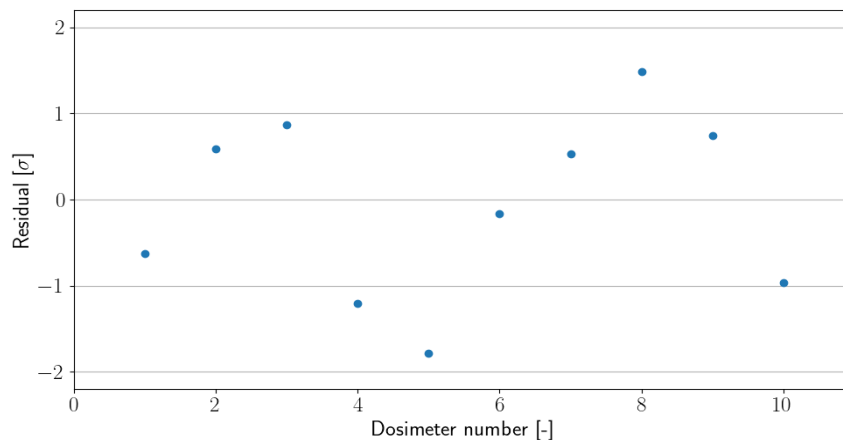


Figure 3. Residual of the ten $^{197}\text{Au}(n, g)$ dosimeters reaction rates of the *lattice model* with respect to the *cuboidal model*.

3. CONCLUSIONS

The analysis of the transmission experiments of PETALE requires a high resolution modelling in order to suppress as much as possible geometrical biases. It is associated with full uncertainty propagation using Total Monte-Carlo, to finally provide results that would adequately constrain nuclear data, e.g., using the Bayesian Monte-Carlo data assimilation method.

As PETALE transmission experiments take place in the periphery of the CROCUS reactor, Variance Reduction was already necessary to obtain sufficient statistics in the small dosimeters' volumes in the simplified model used for design purposes. At the analysis stage, the addition of numerous structural parts, elemental compositions, and voxelization of reflectors sheets, has the consequence of drastically increase the total computation time. The profiling highlights the significant computational cost of surface transformations. The factorization as a universe transformation of common transformations already allows to divide the computational time by a factor 2.5. The price to pay is only a moderate increase in the complexity of the geometry definition, especially for specific usage such as geometry perturbations.

The voxelization of PETALE's reflector using Serpent 3D lattices instead of standard cells is tested. This test proves successful as it reduces to zero the computational cost of the eight reflectors voxelization in 121 zones each. The profiling shows that the use of lattices significantly decreases the time the code pass searching for particles positions and computing distances to surfaces. Finally, in order to further decrease the computational cost of the geometry refinement, an overall redefinition of the model is performed making extensive use of Serpent universes and nested universes. The refined and final model is also considered satisfactory as the Figure Of Merit is only decreased by 15 % compared to the design model, although it includes more details. The model is now ready to perform simulations that will be compared to the PETALE campaign experimental results.

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