PARCS Few-group Homogenized Parameters Generation using Serpent Monte Carlo code at the CROCUS Reactor

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Abstract. The few-group parameters (macroscopic cross sections, discontinuity factors, kinetic parameters, etc.) required for the solution of the neutron diffusion equation by core simulators are traditionally generated from two-dimensional deterministic lattice calculations. However, the use of continuous energy Monte Carlo techniques to generate these few-group parameters has advantages for reactor cores with irregular geometries and also when 3-D cross section spatial collapsing is required due to non-negligible axial neutron leakage. This approach is very attractive to the CROCUS reactor at EPFL since its core presents peculiar characteristics: two incongruous fuel lattices with a core that is partially submerged in water.

The long-term objective of the project is to build and validate a coupled TRACE/PARCS model of the CROCUS reactor. The work presented in this document deals with few-group parameters generation for the CROCUS reactor using Serpent Monte Carlo code and SerpentXS python wrapper. A Serpent model of the reactor was developed and verified against a preexisting MCNP reference model, achieving 17 pcm difference in terms of k_{eff}. The Serpent model was later used along with SerpentXS python script to generate the two-group parameters required by PARCS code. Several Serpent homogenization schemes and methods were applied and preliminary tested in a PARCS model of the reactor. Preliminary results suggest that the best available scheme is the so-called *full-scale* which returned a difference, in terms of k_{eff}, of 395 pcm with respect to Serpent criticality calculations. An attempt to compute the control rod worth in PARCS (394 pcm) showed discrepancies in the order of 10% with respect to Serpent (358 pcm).

1. Introduction

The primary interest in reactor analysis is to be able to model day-to-day steady state operation of the reactor core, or to model brief periods of time during which the reactor is experiencing operational transient due to an unexpected insertion or removal of reactivity. Although direct full core transport calculations (such as DeCART [1], nTRACER [2] and MPACT [3]) are becoming important with the increase of computational power, the full analysis of a nuclear reactor core currently implies using the traditional multi-step methodology [4]. This approach begins with *lattice physics* to condense and homogenize spatially and spectrally the microscopic cross-section data into the structure needed for coarser-level codes (i.e., few-group parameters generation), and concludes with the *core physics* calculations to perform steady state and transient full core reactor calculations.

Traditionally, few-group parameters generation for full core reactor simulators (such as PARCS) has been done using deterministic lattice physics codes. However, the use of continuous-energy Monte Carlo (MC) codes to generate few-group parameters can become an interesting option when dealing with reactor types that lie beyond the capabilities of conventional deterministic lattice physics codes [5]. CROCUS reactor characteristics make this methodology interesting as its core present two incongruent fuel lattices with a water gap in between, with no possible subdivision of the core in smaller sections (such as fuel assemblies).

Serpent, a Monte Carlo code developed at VTT [6], has been specifically designed for group parameters generation and other lattice physics applications. Serpent represents the state-of-the-art for Monte Carlo lattice physics, and has been chosen to provide the nodal code PARCS with the few-group parameters in the framework of development of a coupled TRACE/PARCS model for the CROCUS reactor.

This paper describes the methodology applied for few-group parameters generation on the CROCUS reactor using Serpent 1.1.19, and also provides a comparative assessment of different homogenization schemes.

2. The CROCUS reactor

The CROCUS reactor, operated by the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland is a two-zone uranium-fuelled, H_20-moderated critical research facility. It can be classified as a *zero power* reactor, with a maximum allowed power of 100 W. The core is approximately cylindrical in shape with a diameter of about 60 cm and a height of 100 cm. The reactivity in the CROCUS reactor is controlled by the water level, which can be adjusted with an accuracy of ±0.1 mm [7].

There are two different kinds of fuel rods within the CROCUS reactor core (see Fig. 1). The central zone is fuelled with 336 $U0_2$ fuel rods (1.806 wt.%-enriched), which are thinner rods with a square lattice pitch of 1.8370±0.0002 cm. The peripheral zone is loaded with 172 thicker fuel rods (0.947 wt.%-enriched) with a pitch of 2.9170±0.0002 cm. All fuel rods have an aluminum cladding and are maintained in a vertical position by the upper grid and lower grid plates spaced 100 cm apart (see Figure 2). Because of the different pitches used, the two fuel zones are separated by water gaps, as appreciated in Figure 1. The core is located in an aluminum water tank of 130 cm diameter and 1.2 cm thick. Light water (H_2O) is used as moderator and reflector. Figure 2 provides a view of the reactor structure, the water tank, support plates and fuel rods.

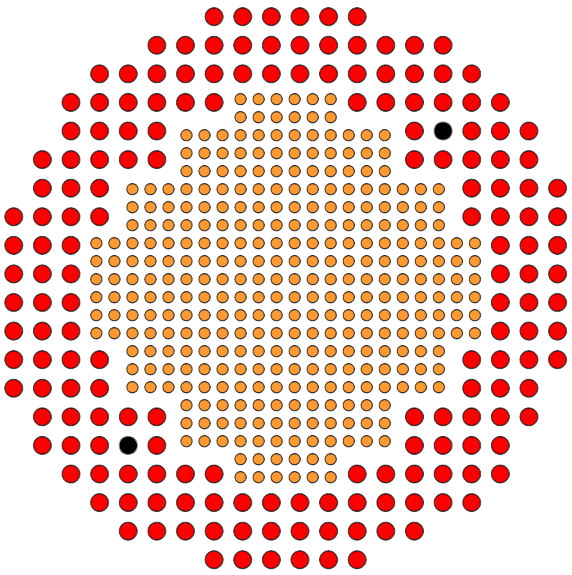

FIG. 1. CROCUS core fuel lattices - UO_2 fuel (orange), U-metal fuel (red), control rods (black)

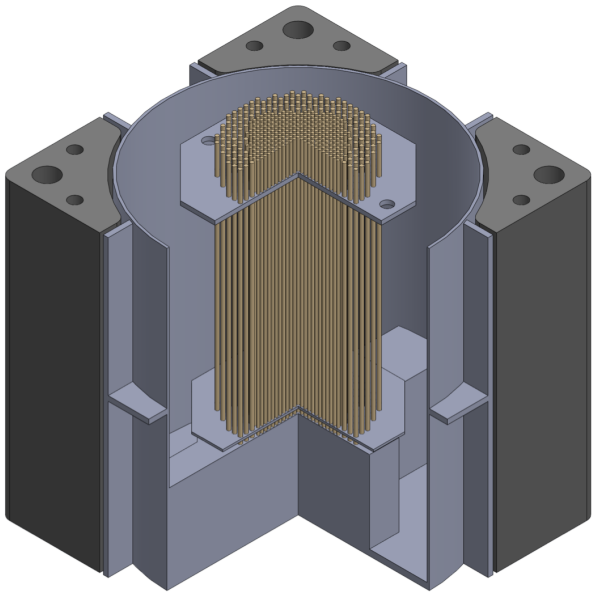

FIG 2. Isometric view of CROCUS reactor structure and core.

3. Few-group parameters generations

The main motivation for using the continuous-energy Monte Carlo method for lattice physics calculations in the CROCUS reactor, is its inherent capability to handle geometry and interaction physics without major approximations. When used for spatial homogenization, Monte Carlo codes also have the advantage of being able to model the full-scale heterogeneous problem, which represents the best available reference solution for the calculation scheme.

The purpose of this section is to present three different approaches taken for the two-group parameters generation using Serpent code. A full core Serpent model for the CROCUS reactor model was developed and verified against a preexisting MCNP5 model. While the statistical accuracy in both Serpent and MCNP is of 10 pcm in the 95% confidence interval (2σ), the difference in k_{eff} between both codes is of 17 pcm, indicating that there is a difference in the models. However, this difference is negligible since the uncertainty due to nuclear data library is of 500 pcm.

Since it is currently beyond Serpent 1.1.19 ability to perform branch calculations and print cross sections into a PARCS compatible format, Serpent was coupled to SerpentXS python script [8]. This allowed generating branch cases and post processing the two-group parameters generated by Serpent to be PARCS readable.

Serpent 1.1.19 and ENDF/B-VII nuclear data library were used for all Monte Carlo simulations. These calculations were run using 800 cycles of 10^8 neutrons each, returning a final statistical uncertainty below eight pcm for eigenvalues calculations and 0.01% for two-group parameters generation.

Serpent has the ability to produce diffusion coefficients using the traditional P1 approximation but it has also implemented a B1 fundamental mode methodology to correct diffusion coefficients based on an approximate leakage spectrum [5]. In this paper, both methods were used to compute the diffusion coefficient. The traditional P1 method defines the group diffusion coefficient as

$$D_g = \frac{1}{3\Sigma_{tr,g}} = \frac{1}{3(\Sigma_{t,g} - \bar{\mu}_{0,g}\Sigma_{s0,g})} \tag{1}$$

Where D_g is the group diffusion coefficient, $\Sigma_{tr,g}$ the macroscopic transport cross section, $\Sigma_{t,g}$ the total macroscopic cross section, $\bar{\mu}_{0,g}$ the average cosine of the scattering collision angle and $\Sigma_{s0,g}$ the zeroth moment of the scattering cross section.

On the other hand, when the B1 mode is activated in Serpent, it solves the B1 equations [9] where k_{eff} is iterated to unity to get a better approximation of the neutron energy spectrum, resulting in the *critical flux* (φ_g) and current spectrum (J_g). Then, the diffusion coefficient is computed as

$$D_g = \frac{J_g}{|B|\phi_g} \tag{2}$$

Where B is the buckling.

In addition to the B1 definition of the diffusion coefficient, Serpent 1.1.19 has the ability to use the *critical flux spectrum* (φ_g) (resulting from the B1 equations) to re-homogenize the cross sections into leakage corrected cross sections. However, this option was not used in this work as all cross sections have been homogenized using the *infinite spectrum*.

The first homogenization scheme involves solving the *full-scale* problem, where the whole CROCUS core is modeled assuming neutron leakage from the system, i.e., zero incoming current boundary conditions in all three directions. A set of four homogenized cross sections are generated using Serpent's ability to select universes for homogenization. Figure 3 shows the way universes are handled to generate few-group parameters using the *full-scale* homogenization scheme. The advantage of this approach is that the flux used for the spectral homogenization (i.e., for conserving reaction rates) is a better approximation since the whole core geometry is being considered.

Both B1 and P1 methods have been used to compute the diffusion coefficient in the *outer fuel* and *inner fuel* regions. However, since the B1 method cannot be utilized in a region where a critical spectrum is not applicable, only the P1 method has been used for the reflector and control rods region.

All homogenization schemes presented in this work generate, essentially, 2-D cross sections since they do not vary along the axial direction.

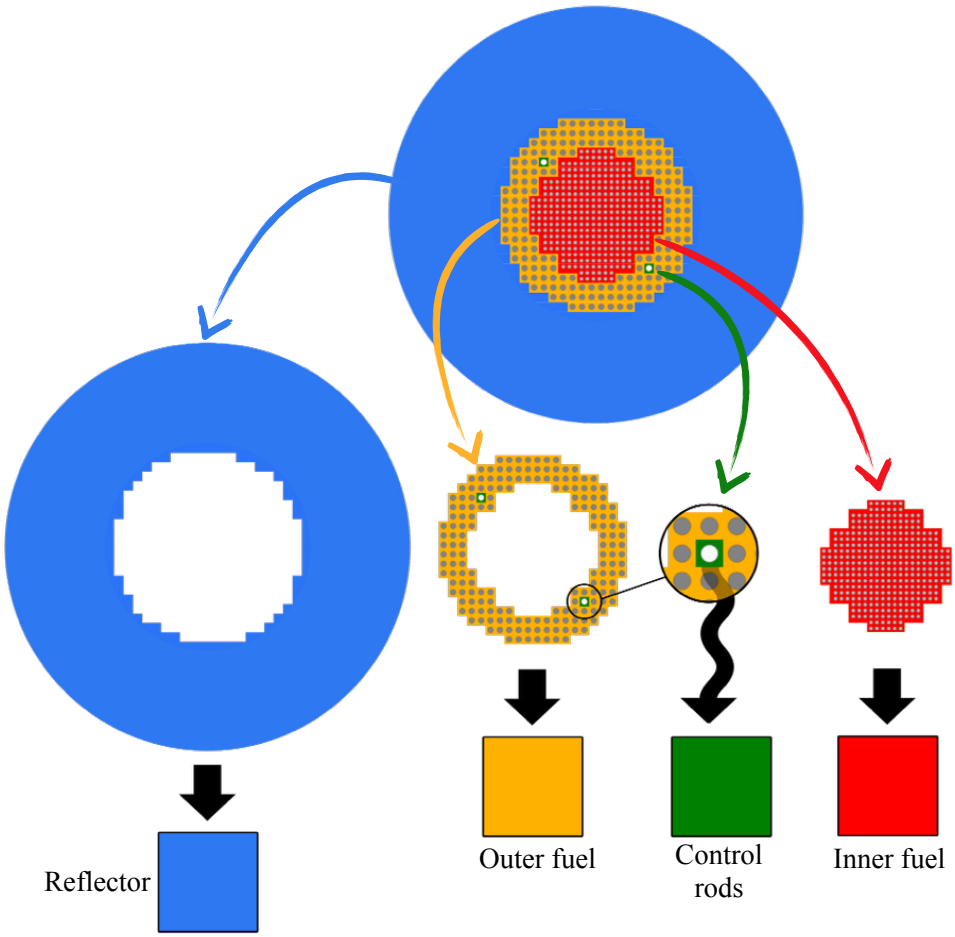

FIG. 3 Full-scale homogenization scheme

The second homogenization scheme implies subdividing the core into nine sections and homogenizing each area separately using reflective boundary conditions in *x* and *y* directions. Axial leakage is taken into account. Each homogenized region corresponds to an area equivalent to four by four U-metal pin cells as illustrated in Figure 4. Although the CROCUS reactor core is not arranged in fuel assemblies, this homogenization scheme is similar to that performed at assembly level in other reactors.

The reflector region cross-sections are obtained using an array of fuel pins (representing the interface between the core and reflector) to provide the reflector region with neutrons (see Fig. 4). Moreover, control rods are incorporated in region 3 (see Fig. 4) and homogenized with fuel and reflector.

In this homogenization scheme, diffusion coefficients have also been computed using P1 and B1 definitions (Eq. 1 and 2). Due to the absence of fissile material in the reflector region, the diffusion coefficients were computed using only the P1 definition.

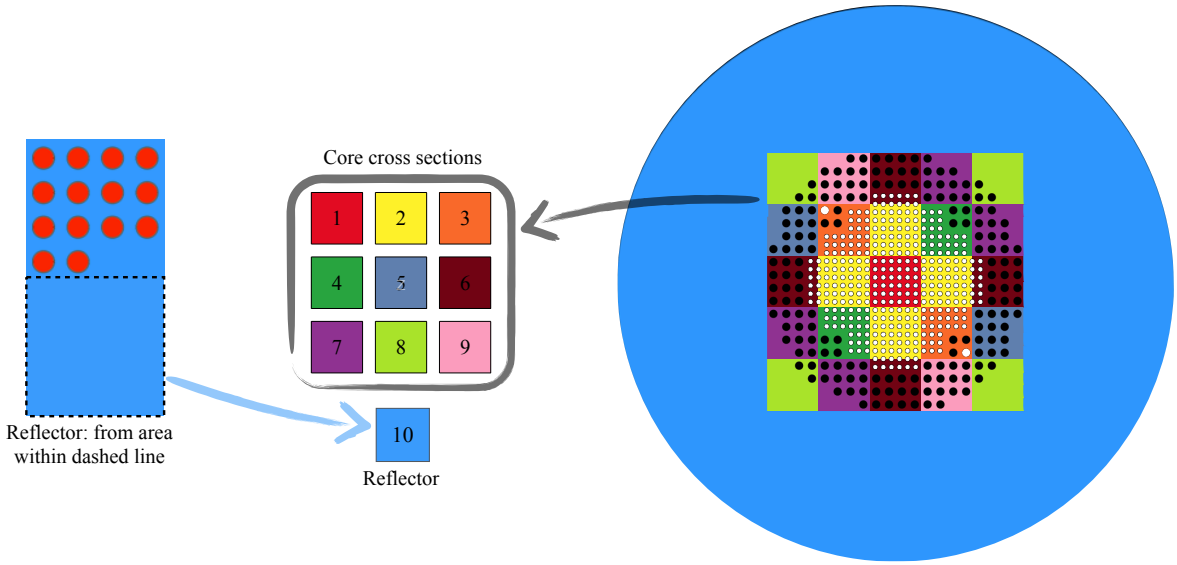

FIG. 4 "Assembly-level" type homogenization scheme

The third homogenization scheme is carried out at a *pin cell level* (see Fig. 5) using reflective boundary conditions in all directions. However, special treatment has been taken over the control rod and reflector regions since they need a source of neutrons for the spectral homogenization. Accordingly, the geometry used for control rods homogenization includes eight U-metal fuel pins and one control rod in the center as shown in Figure 5. Also, the reflector region was homogenized in a similar way to the *assembly-level* type scheme, but scaled down to a few pins. The disadvantage of the *pin cell level* homogenization scheme is that it ignores the water gap between the lattices and its influence upon the flux spectrum. Axial leakage is not taken into account, i.e., a 2-D geometry was used for the homogenization.

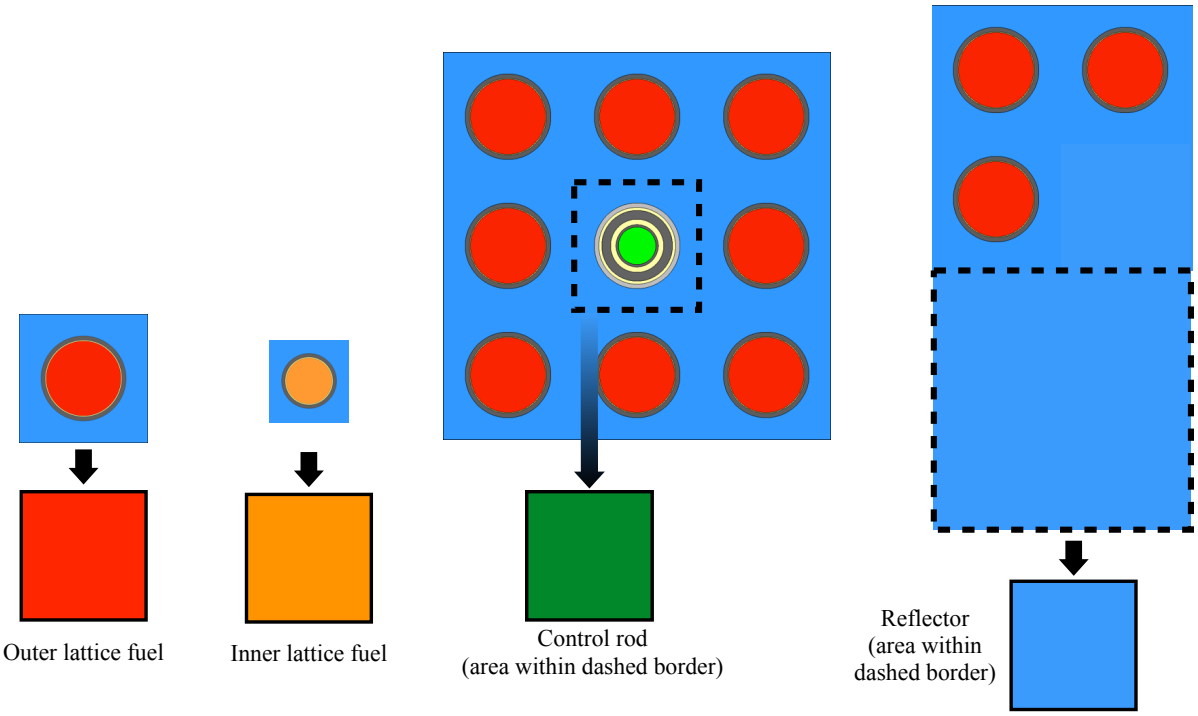

FIG. 5 Pin-cell level homogenization scheme

4. Whole core calculations with PARCS

Nodal methods are widely used for whole-core reactor physics calculations. Each node normally corresponds to a small portion of the reactor core (e.g. to an axial slice of fuel assembly) for which homogenized cross sections have first been obtained. PARCS is a multi-group nodal diffusion code developed by the U.S. NRC for 3-D steady state and transient analyses. The few-group parameters in this whole-core study were generated using the Serpent code and the various homogenization schemes presented earlier.

Two PARCS models of the CROCUS reactors were built according to the needs of the different homogenizations schemes. In both PARCS models, the node size was chosen to correspond to one metallic uranium fuel-pin cell (2.9170 cm x 2.9170 cm). Axially, the core was subdivided into 25 nodes of 3.8088 cm each, matching the 95.22 cm of active core modeled in Serpent. PARCS models take into account 47 cm of water below the core, which is also being modeled in Serpent. The Serpent geometry served as reference for the design of PARCS models. Figure 6 shows a top view of the different geometries used for the PARCS and Serpent models.

In reality, the total length of the fuel rods is 100 cm, yet, only 95.22 cm are submerged in water (this corresponds to the experimentally determined critical water level). Thus, there is an extra 4.78 cm of fuel rods moderated by air that is taken into account in Serpent model. However, this was not considered in any PARCS model, as it is believed to have a negligible effect in terms of k_{eff} or power shape.

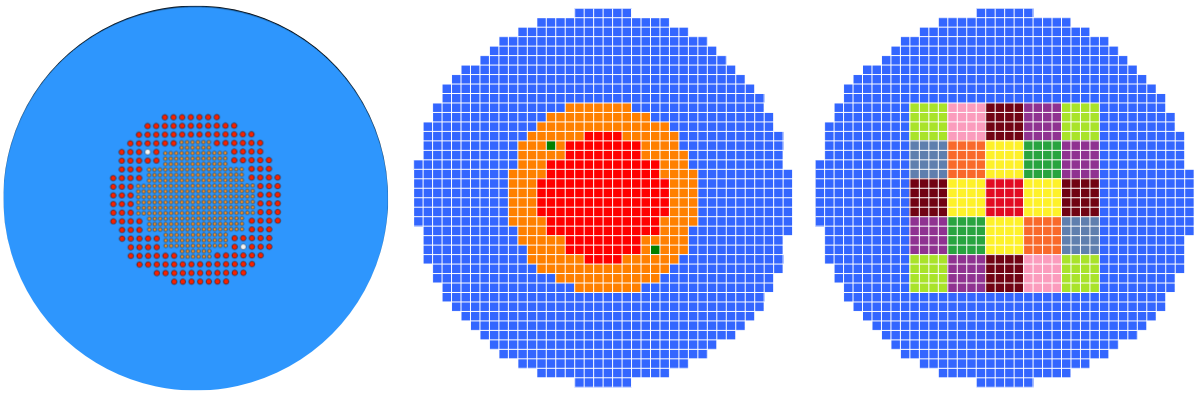

FIG. 6 Serpent vs. PARCS geometries for different homogenization schemes.

5. Serpent vs. PARCS static simulations

Serpent model is used as reference for the comparison of the different homogenization schemes presented in Section 3. In a first comparison exercise, the effective multiplication factors and control rods reactivity worth are evaluated and presented in Table 1. Since Serpent multiplication factor is very close to unity, no normalization was required and the difference was computed as

$$\Delta k_{eff} = k_i - k_{Serpent} \tag{3}$$

Where *i* denotes different PARCS models and homogenization methods.

The control rod worth was computed in Serpent as the k_{eff} difference between a model containing the control rods fully withdrawn, and the one with control rods fully inserted. In PARCS, the control rod worth was computed in a similar way, using a card that allows inserting or withdrawing the control rods. Finally, the percent difference reported in Table 1 was computed from the following expression

$$\Delta worth_{\%} = \frac{worth_i - worth_{Serpent}}{worth_{Serpent}} \times 100 \tag{4}$$

TABLE I: k_{eff} and control rod reactivity worth comparison for Serpent and PARCS

		Eigenvalue		**Control rod worth**	
	Model	k_{eff}	Δ_{keff} *(pcm)*	*Worth (pcm)*	*ΔWorth/Worth (%)*
Serpent 1.1.19		1.00184 ± 8 pcm	-	358	-
PARCS	Full-scale B1	1.00580	395	394	10%
	Full-scale P1	1.02766	2582	354	-1%
	Assembly-level B1	0.99531	-653	531	48%
	Assembly-level P1	1.02144	1960	537	50%
	Pin-level B1	1.02586	2402	387	8%
	Pin-level P1	1.04901	4717	345	-4%

The results shown in Table 1 suggest that the *full-scale* scheme with the B1-defined diffusion coefficient is the best in predicting k_{eff}. Also, the table clearly shows that the choice of B1 or P1 methods for the diffusion coefficient is critical since selecting one or the other will return considerably different multiplication factors (~2000 pcm difference). However, a k_{eff} comparison is not enough to tell which homogenization scheme is the most accurate one.

An additional comparison exercise was focused on fuel element power distributions. Due to the mismatch between PARCS nodes and the CROCUS reactor inner lattice fuel pins (see Fig. 9), only the Serpent outer lattice power can be compared against PARCS nodal power. Also, the *assembly-level* scheme was excluded from this comparison since the reactor core was modeled as a square block (recall Fig. 6).

Serpent fission power was extracted using an *x* and *y* mesh with detector tallies with a fission multiplier. While the mesh in *x* and *y* is as represented in Figure 9, in the axial direction (*z*) there is a single node covering the active part of the core up to the water level (95.22 cm). To make Serpent power comparable with PARCS power maps, each node was normalized with respect to the average power of all nodes as follows

$$\bar{P}_{i,Serpent} = \frac{P_{i,Serpent}}{\left\langle P_{Serpent} \right\rangle} \tag{5}$$

Where $\left\langle P_{Serpent} \right\rangle$ is the average power.

On the other hand, PARCS nodal power is already normalized (as in Eq. 5) and printed in the output file. This file contains a 2-D power map, resulting from the axial average of the 25 radial power maps. Finally, the difference between Serpent and PARCS radial power is computed as

$$\%diff. = \frac{\bar{P}_{i,Serpent} - \bar{P}_{i,PARCS}}{\bar{P}_{i,Serpent}} \times 100 \tag{6}$$

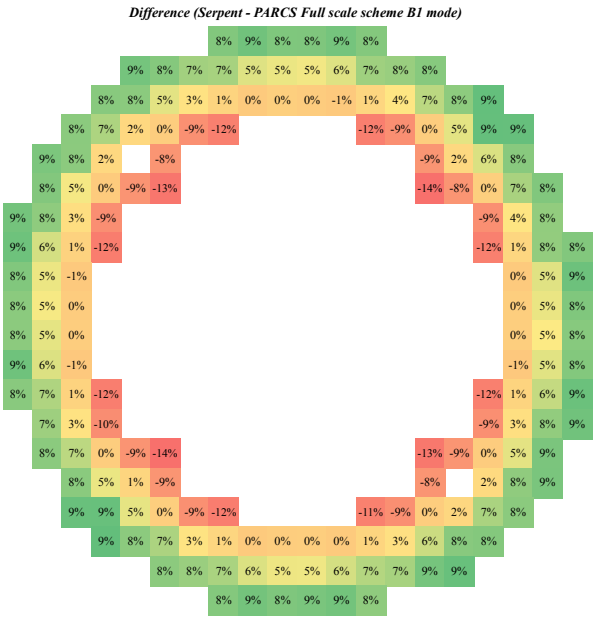

FIG. 7. Nodal power % difference for Full-scale scheme

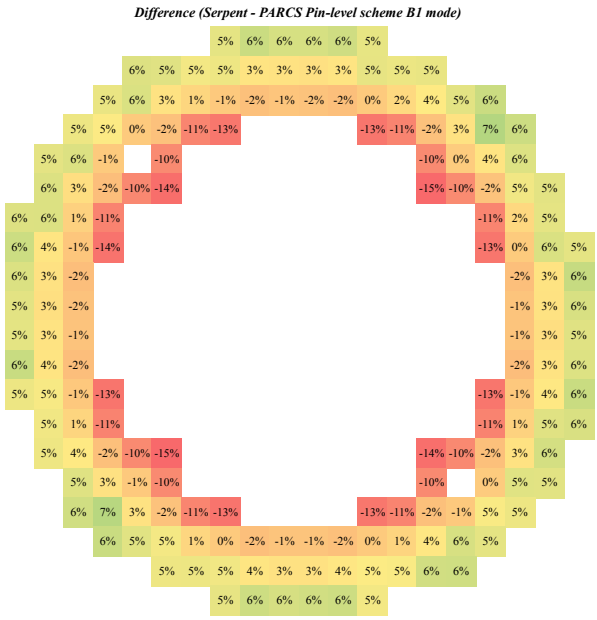

FIG 8. Nodal power % difference for pin-level scheme

Figures 7 and 8 show the outer lattice power comparison between Serpent and PARCS for *full-scale* and *pin-level* homogenizations schemes respectively. As mentioned earlier, due to the fuel pin/nodes mismatch in the inner lattice, only a comparison over the outer lattice has physical meaning. It should be noted that even though the *pin-level* scheme over-predicts the multiplication factor by more than 2000 pcm, its prediction of radial power distribution is more accurate than that of the *full-scale* scheme. The author believes that this unexpected agreement could be caused due to compensation of errors.

The *full-scale* scheme with B1 diffusion coefficient is believed to be the best available scheme overall since it is able to predict the k_{eff} within 395 pcm, control rod reactivity worth with 10% difference and power shape with an accuracy below 14%. However, this results are not completely satisfactory, as 14% discrepancy in power prediction is too large.

The next section is therefore devoted to the *full-scale* scheme, particularly on the difference between B1 and P1 methods for computing diffusion coefficients. Thus, Serpent will be hereafter not considered and only PARCS results will be presented.

A radial power comparison between P1 and B1 methods for diffusion coefficients was performed for the whole core as shown in Figure 10. A slice in the *x* direction was taken (see dashed line in Fig. 10) to provide a profile view of the radial power shape.

Figures 11 and 12 show the radial and axial power profiles comparison respectively. Radially, it becomes clear that the B1 method predicts a flatter power profile. Axially, the only noticeable different is in the bottom of the core due to the presence of water that reflects neutrons back to the system.

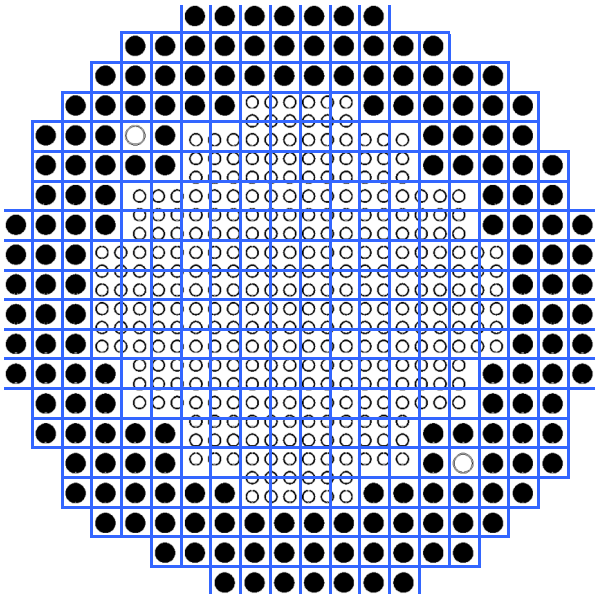

FIG. 9 Mismatch between PARCS nodes and Inner lattice fuel pins

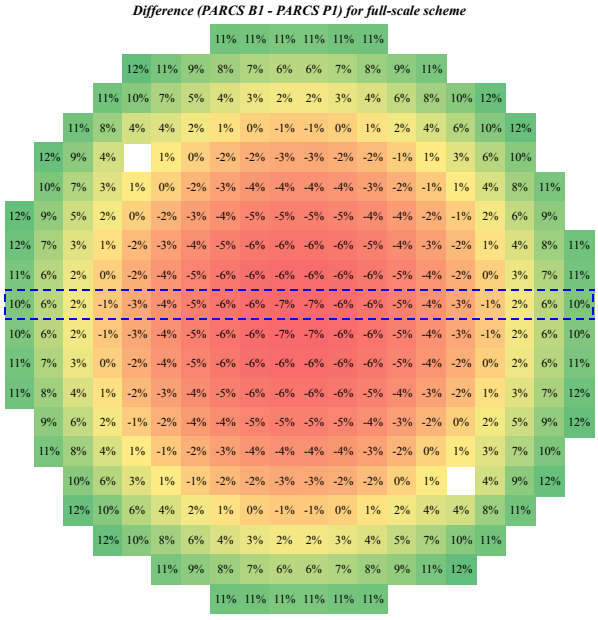

FIG. 10 B1 mode vs P1 approximation nodal power difference for full-scale scheme

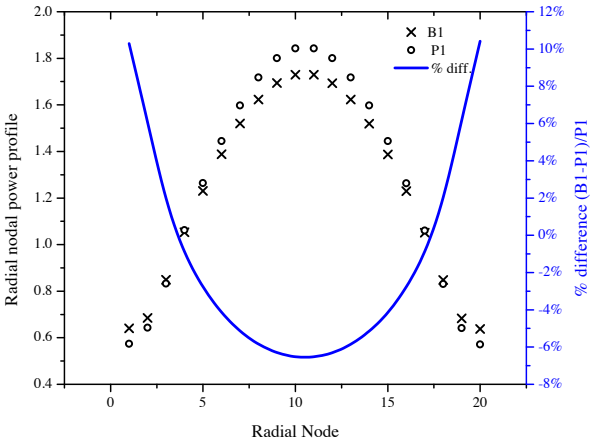

FIG. 11 B1 mode vs. P1 approximation radial power comparison for full-scale scheme

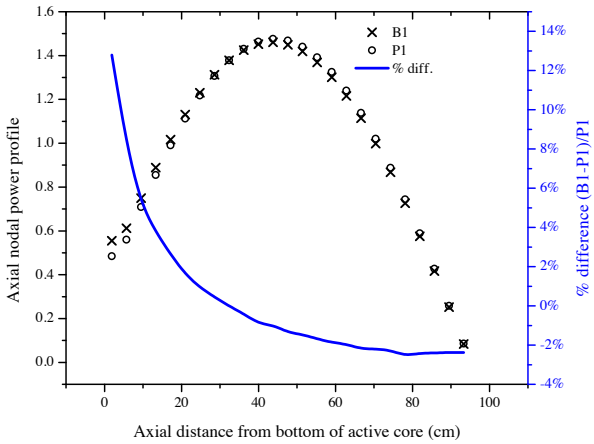

FIG. 12 B1 mode vs. P1 approx. axial power comparison for full-scale scheme

5. Conclusions

In this paper, the use of Monte Carlo techniques to generate few-group parameters has been studied. The Monte Carlo code Serpent was used to model the CROCUS reactor at EPFL and to provide the nodal code PARCS with two-group parameters. Different homogenization techniques have been tested with PARCS code and compared against Monte Carlo solutions. Focus has been made over B1 and P1 methods for computing diffusion coefficients; both available in Serpent 1.1.19 code. The best overall homogenization technique resulted to be the so-called *full-scale* scheme with B1 diffusion coefficient definition. With this technique, predictions with respect to Serpent were within 400 pcm for k_{eff}, 10% for control rods and 14% for power distribution.

Due to the high leakage potential of small reactor cores such as the one present in CROCUS, it was found that the diffusion coefficient (i.e., choice of B1 or P1 methods in Serpent) plays a critical role in eigenvalue and power shape predictions.

The preliminary results are encouraging and further investigations will be carried on, typically with a more in depth analysis of fundamental differences between P1 and B1 methods for the determination of the diffusion coefficients. The development of an adequate homogenization scheme will be continued until power, eigenvalue and control rod worth are predicted with an acceptable degree of accuracy. Also, the complete understanding of differences between schemes in terms of eigenvalue and power shape predictions are planned as future work along with experimental validation of the PARCS model.

6. References

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