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Progress toward the development of a high-fidelity neutronic model of MARVEL using Griffin

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ABSTRACT

The Microreactor Applications Research Validation and Evaluation (MARVEL) is a 100 kW_{th} microreactor envisioned to start operations at Idaho National Laboratory (INL) in early 2025. This paper is focused on the development of a high-fidelity neutronic model of the MARVEL reactor using Griffin. In particular, the step-by-step verification procedure against Serpent reference calculations is reported here. The comparisons are here performed in terms of effective multiplication factor and pin-wise fission source spatial distribution. The neutronic model here presented will be the foundation of a multiphysics transient model that will be used to validate NEAMS tools against the MARVEL reactor once operational.

Keywords: MARVEL, NEAMS, high-fidelity model, discrete ordinates

1. INTRODUCTION

The Microreactor Applications Research Validation and Evaluation (MARVEL) is a 85-kW_{th} microreactor intended to be operated at Idaho National Laboratory from early 2025 [1]. A 3D rendition of the envisioned reactor is displayed in Fig. 1. The MARVEL core will use Uranium Zirconium Hydride (U-ZrH) for fuel and sodium-potassium eutectic (NaK) for coolant. Reactivity control will be achieved via four control drums with boron carbide (B₄C) absorbing segments inside a beryllium radial reflector. Stirling engines will be used to convert the thermal energy into electrical energy. The MARVEL reactor is envisioned to demonstrate several operating features of microreactors, including the investigation of diverse electrical and thermal applications and the evaluation of autonomous technology.

In this paper, the progresses made towards the development of a high-fidelity neutronic model of MARVEL using Griffin are reported [3]. In particular, the paper focuses on verification of the steady-state neutronic model against Serpent reference calculations. This model will lay the foundation for a comprehensive verification and validation (V&V) activities against the physical system starting in Fiscal Year 2025. This collaborative V&V exercise across the Nuclear Energy Advanced Modeling and Simulation (NEAMS) and the Microreactor Program (MPR) programs is intended to be mutually beneficial, with data being provided to NEAMS and code capability being provided to the MRP to advance the deployment of microreactor technology.

The remainder of the paper is structured as follows. Section 2 describes the model, including cross sections preparation, meshing, and full-core solution method. The results of the analyses are reported in Section 3. Finally, summary and conclusions are drawn in Section 4.

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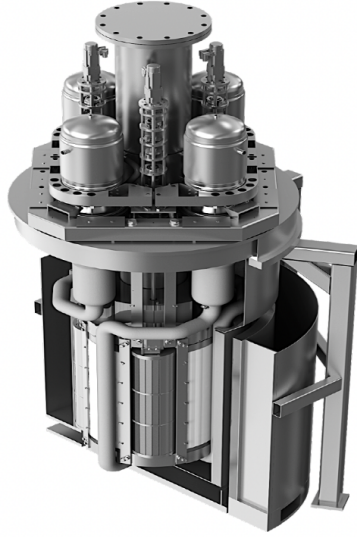


Figure 1. 3D rendition of the MARVEL reactor concept from [2].

2. METHODOLOGY AND CODES

The verification of the Griffin neutronic model against Serpent [4] was performed using a step-by-step approach consisting of defining three problems of increasing complexity from the full reactor geometry. In this section we describe the codes and methodology used to generate the full-core 3D problem (*i.e.*, P3). Specific information on the problems, denoted as P1–3 will be provided in Section 3.

2.1. Meshing the Geometry

The neutronic mesh was generated using the reactor module in MOOSE [5, 6]. The reactor module aims to enhance MOOSE meshing capabilities for nuclear reactors, eliminating the need for reliance on external codes. The MARVEL geometry generated with the reactor module is shown in Figures 2a–b, where a radial view of the core mid-plane and a 3D view of the core geometry are reported, respectively. As a demonstration of the flexibility of the reactor module to handle irregular geometry, the ability to mesh the quadrilobed external radial reflector is showcased in Figure 2 (purple sub-domain). The generated 3D mesh contains 1,152,312 elements, including 21 axial layers and 54872 elements per axial layer. In this work, the *BeO* inner reflector geometry is approximated using a polygonal curve rather than a smooth curve following the curvature of the pins (as shown in the Serpent model in Fig. 3. However, the mass of reflector is preserved by adjusting the density of the material to match the mass of *BeO* in the Serpent input.

2.2. Multigroup Macroscopic Cross Sections

Serpent (v.2.1.32) [4] was used to generate the multigroup macroscopic cross sections. Serpent is a 3D Monte Carlo code developed by VTT to enable the modeling and simulation of neutron and photon transport in nuclear reactors and the calculation of lattice parameters (*i.e.*, multigroup cross sections and point kinetic parameters). The use of Serpent for cross sections generation was motivated by the existence of a mature workflow to import Serpent-generated cross sections to Griffin. Future work will be devoted to investigating the use of Shift [7], that is a NEAMS code, and OpenMC [8] for the cross sections tabulation step. The cross sections were generated using the modified Hansen-Roach energy structure. The latter was utilized

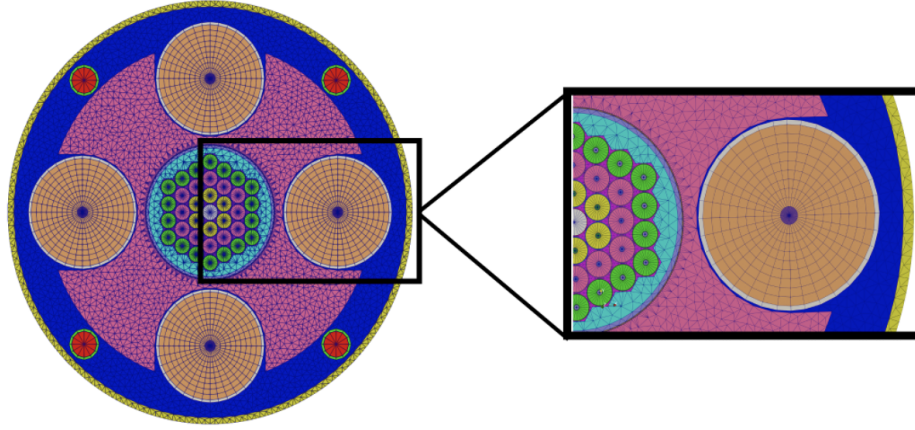


Figure 2. (a) View of mesh at the mid-plane and zoom-in for the inner reflector (in teal) showing the polygonal approximation.

to generate the cross sections fed into the SNAP8-ER Griffin model in Ref. [9]. This energy structure was chosen based on the similarities between MARVEL and SNAP8-ER in terms of material and dimensional specifications (*e.g.*, fuel type, reflector material, dimensions, etc...). For the sake of completeness, the boundaries of the group structures are reported in Table I. For verification purposes, the reference steady state point is defined by imposing a temperature of 900 K for fuel, 600 K for the NaK and 300 K for the other components.

Table I. Energy group (upper) boundaries for the 18-group structure used in the Griffin model.

Group	Energy (MeV)	Group	Energy (MeV)
1	$2.00 \times 10^{+1}$	11	9.70×10^{-5}
2	$1.00 \times 10^{+1}$	12	3.00×10^{-5}
3	3.00×10^0	13	1.00×10^{-5}
4	1.40×10^0	14	3.00×10^{-6}
5	9.00×10^{-1}	15	1.00×10^{-6}
6	4.00×10^{-1}	16	4.00×10^{-7}
7	1.00×10^{-1}	17	1.00×10^{-7}
8	1.70×10^{-2}	18	1.00×10^{-8}
9	3.00×10^{-3}	19	5.00×10^{-9}
10	5.50×10^{-4}		

2.3. Discrete Ordinates Neutronic Model in Griffin

Griffin is a MOOSE-based reactor physics deterministic code for steady state and transient neutral particles' transport [3]. Due to its general nature, Griffin contains several solvers for the neutron transport equation and its lower order approximations, including diffusion. In this work, the neutron transport equation is discretized in space using the upwind discontinuous finite element method (DFEM), while the angular dependence is accounted for using the discrete ordinates method, commonly denoted as S_N method. The DFEM- S_N method was first introduced in Reed and Hill in 1973 to enable neutron transport modeling and simulation on unstructured mesh. The DFEM- S_N solver in Griffin was chosen to solve the neutron transport equation in MARVEL because of the small core dimensions that make streaming and, therefore, neutron

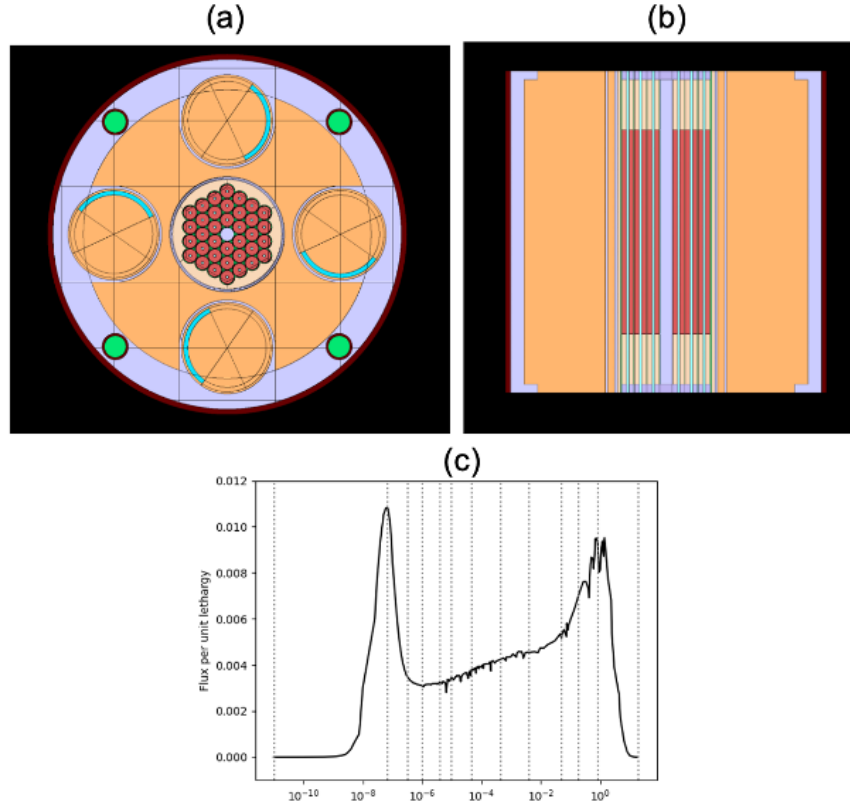


Figure 3. (a) Radial and (b) axial view of the MARVEL Serpent model. (c) Spectrum per unit lethargy for the full reactor (black line) and upper boundaries for energy group structure (dotted vertical line).

leakage a crucial term to capture in reactor physics calculations of this core. Also, the small dimensions of the core allows the problem to be solved with a reasonable amount of computational resources. In fact, the DFEM- S_N discretization scheme, in conjunction with the asynchronous parallel sweeper implemented in Griffin for inverting the streaming operator, enables efficient performance of neutron transport calculations in a parallel fashion on an unstructured mesh. Additional performance improvement can be achieved by deploying the Coarse-Mesh Finite Difference (CMFD) acceleration technique, that was demonstrated to be able to decrease the total number of transport sweeps, and, therefore, the execution time of the simulation [10].

3. RESULTS AND DISCUSSION

As discussed in Section 2, the Griffin neutronic model is verified against Serpent using a set of three problems of increasing difficulty and denoted as P1–3.

3.1. Error metrics

In this paper, the comparison is performed only in terms of effective multiplication factor and pin power spatial distribution. To measure the difference between the Serpent reference and the Griffin calculations, we use the following error metrics:

- For the effective multiplication factor, denoted here as k , we define the relative error in percent per mille (pcm) as:

$$\frac{\delta k}{k} = \frac{k_{griffin} - k_{serpent}}{k_{serpent}} \times 10^5, \quad (1)$$

where $k_{griffin}$ and $k_{serpent}$ denote the effective multiplication factor computed by Griffin and Serpent, respectively.

- For the pin power distribution, the error is measured as:

$$RMSPE_P = \sqrt{\frac{\sum_{n=0}^N (P_n^{griffin} - P_n^{serpent})^2}{N}} \times 100, \quad (2)$$

where N is the number of pins, $P_n^{griffin}$ is the power computed by Griffin for pin n and $P_n^{serpent}$ is the power computed by Serpent for the n^{th} pin. The pin-wise maximum error is also reported and denoted by e_{max}^P .

3.2. Verification exercise

Geometrical representation for problems P1 and P2 are shown in Figure 4, where Griffin mesh and Serpent model geometry are juxtaposed. P3 geometry is not shown since the problem was described in Section 2.

1. **P1** is a 2D pseudo unit-cell, in which a clad U-ZrH pin radial cross section (in red) is surrounded by NaK coolant (in green). The geometry of the pseudo unit cell is reported in the first row of Figure 2. Reflective radial boundary conditions are imposed to the 2D problem.
2. **P2** is 2D core problem, formed by a radial cross section of the 3D MARVEL core at the mid-plane. Vacuum boundary conditions are imposed radially. The geometry of the 2D core is represented in the second row of Figure 4.
3. **P3**. The 3D full-core problem is the complete MARVEL problem described in Section 2. The radial axial view of the Serpent geometry together with the 3D core mesh is displayed in the last row of Figure 4.

Table II reports the relative error in multiplication factor, the $RMSPE_P$, the maximum error, together with the execution time for the simulations. All results were obtained using 216 directions for the neutron streaming (3 azimuthal, 9 polar per octant). Linearly anisotropic scattering is used for all the simulations. No coarse-mesh finite difference acceleration is currently employed. The pin problem was run with 8 computing power units, while the two core problems were simulated using 4 full nodes, using a total of 192 processors. It is noticeable that, in terms of power, all cases are consistently within 2% of the pin-wise power distribution for the core calculations, while the effective multiplication factor is captured within 452 per cent mille (pcm) for the 3D core. The main reason for the current discrepancy is that only one axial zone was used for cross sections generation purposes, therefore, not capturing the axial spectral variations. In the final version of this paper, the number of axial zones used to generate the cross sections will be varied to assess the influence of axial discretization and further reduce the discrepancy between continuous energy and DFEM- S_N models.

4. SUMMARY AND CONCLUSIONS

The MARVEL reactor is expected to start operations at INL in early 2025. In particular, the step-by-step verification procedure against Serpent reference calculations is here reported in terms of effective multiplication factor and reaction rates (*i.e.*, fission rates and absorption rate). The model here presented

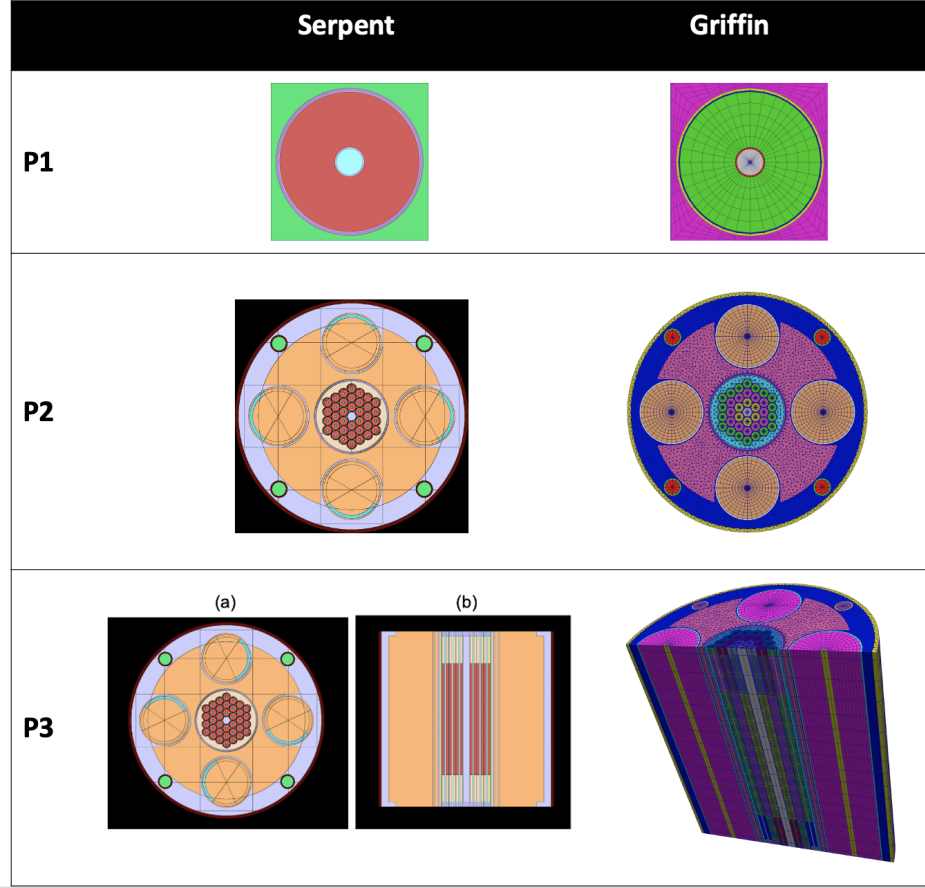


Figure 4. Serpent geometry and Griffin mesh for P1 and P2

Table II. Comparison of Griffin and Serpent. The uncertainty of the Serpent-computed k_{eff} is 1 pcm for problem P1–P3. The reported uncertainty corresponds to one standard deviation.

Problem	e_P^{max}	$RMPSE_P$	$\delta k/k$, pcm	Run-time, s
P1	N/A	N/A	3	9
P2	$1.7 \pm 0.13\%$	$1.1 \pm 0.11\%$	247	142
P3	$2.1 \pm 0.31\%$	$1.4 \pm 0.24\%$	452	326

will be the foundation of a multiphysics transient model that will be used to validate NEAMS tools against the physical reactor once operational.

It was shown in Section 3 that the effective multiplication factor computed with the DFEM- S_N model agrees with Serpent reference calculations within 500pcm for all cases. The pin-wise power distribution agrees within 1.5% in terms of $RMSPE_P$ for both the 2D and 3D full-core case. Further improvement will aim at bringing the discrepancies down to less than 100 pcm on the 3D full-core model, including using more axial zones for cross sections generation and by further tailoring the group structure to the MARVEL spectrum.

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