Selected VERA Core Physics Benchmarks in OpenMC

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ABSTRACT

High-fidelity reference solutions are essential for modern reactor physics modeling and simulation. In the interest of producing more of these solutions, a tool was written to convert models from VERA to OpenMC. Given a suite of core physics benchmarks, it was found that eigenvalue and power distribution calculations in OpenMC closely matched the benchmark solutions provided by CASL.

INTRODUCTION

CASL is developing a reactor simulation environment known as VERA (the Virtual Environment for Reactor Applications) designed for higher-fidelity modeling and simulation capabilities than are available in the current industry approach. VERA is a high-fidelity multiphysics tool which uses a suite of physics codes, state-of-the-art numerical methods, and validation against operational data to simulate fuel rod and thermal hydraulics performance over the lifetime of a PWR [1].

OpenMC is the open source Monte Carlo neutron transport simulation code developed by the Computational Reactor Physics Group (CRPG) at the Massachusetts Institute of Technology. It was developed as a framework for reactor analysis, and was designed to scale on supercomputers with 100,000+ cores while simulating realistic physics and using modern programming style and data structures [2]. OpenMC takes cross sections in ACE format (such as used by MCNP and Serpent) and windowed multipole format for on-the-fly Doppler broadening converted to HDF5.

VERA comes with a detailed set of core physics benchmarks based on the initial core of Watts Bar Nuclear Plant, Unit 1 (WBN1). Our objectives for this project are to develop a tool to automatically convert benchmark problems from VERA's format, to run a selection of them in OpenMC, and to compare them to the reference solutions provided in the benchmark specifications [3].

METHODS

Vera-to-OpenMC

Each benchmark problem is defined by a single ASCII input deck. A tool called VERAin uses a Perl script to parse the common input deck to XML. The objective of this project was to take the XML files produced by VERAin, create an equivalent model in OpenMC, and verify that the OpenMC results match those of the reference solution.

OpenMC contains a rich Python API to aid in the creation and post-processing of simulations. A tool called Vera-to-OpenMC was written in Python 3 to read the XML from VERAin and exploit the API to create the corresponding geometry in OpenMC. For purposes of this paper, we shall examine sets of four of the HZP core physics benchmarks: *2D pincell*, *2D lattice*, *3D assembly*, and *3D full-core*.

Problem 1, containing the 2D pincell cases, was trivial to convert.

Problem 2, containing the 2D lattice cases, is shown in the figures below. Several of these cases contained burnable poison insertions (Fig. 1) or grid spacers (Fig. 2). The spacers were modeled by placing a border of uniform thickness around each cell in the lattice, preserving the spacer's volume and mass. The grid straps and sleeves were not modeled explicitly in either the reference solution or OpenMC model.

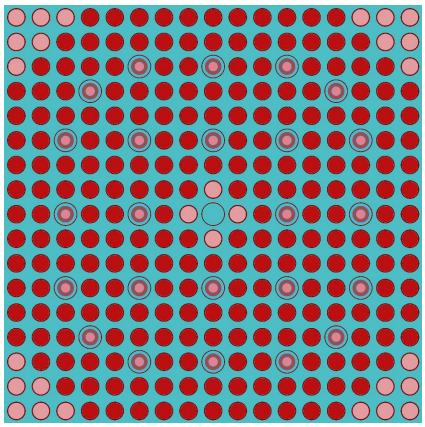


Fig. 1: Problem 2k

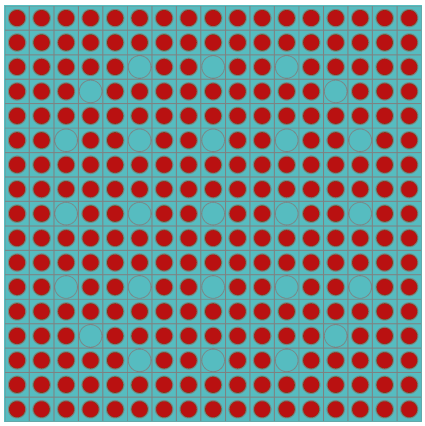


Fig. 2: Gridded lattice from Problem 2q and Problem 3

Problem 3 contains the 3D assembly cases. The assemblies contain spacer grids and burnable absorber insertions like those in the lattice cases within some of the axial zones. In the reference solution, the nozzles were "smeared" with water, with the mass of the original material conserved. CASL assumed the thickness of the core plates and smeared them with water as well, noting that the model should be insensitive

to their values. Nevertheless, the composition of the nozzles and core plates from the reference solution were replicated faithfully in OpenMC. An axial view of one of the assembly cases is shown in Fig. 3 below.

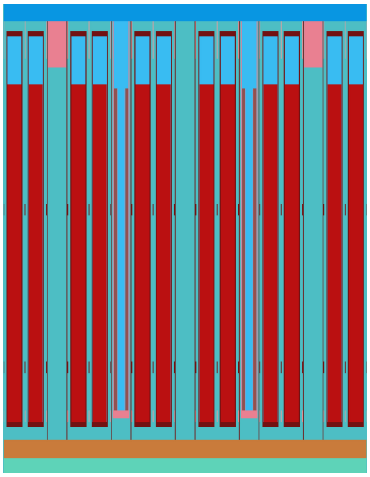


Fig. 3: Problem 3b, axial. (Shortened to show detail.)

There are multiple full-core problems in the benchmark suite, but the models do not vary much from one another except in terms of control rod placement. In addition to burnable poisons, detectors and control rods were featured in these cases. The full radial reflector, core barrel, neutron pads, and pressure vessel were explicitly modeled. A full-core model is depicted in Figure 4.

Cross Section Data

VERA's reference solutions were calculated using SCALE6.2/KENO-VI, a continuous energy Monte Carlo transport code. CASL perfomed each calculation using both ENDF/B-VI.8 and ENDF/B-VII.0 cross-sectional data. We ultimately used the ENDF/B-VII.0 solution to compare results.

In OpenMC, calculations were performed with the ENDF/B-VII.1 data provided with MCNP6. The windowed multipole method [4] was used for Doppler broadening of cross sections. For thermal scattering, continuous-energy $S(\alpha,\beta)$ tables were used for hydrogen in the moderator.

RESULTS

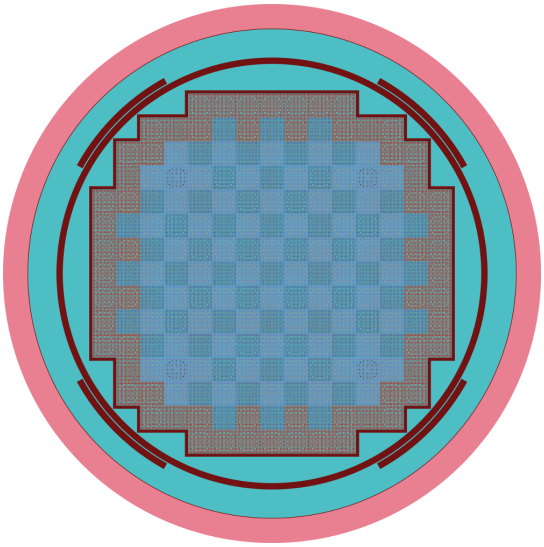
Problem 1

All of the pincell results had differences from the reference solution that were on the order of $\approx$ 20 pcm. The exact numbers appear in Table I in the appendix.

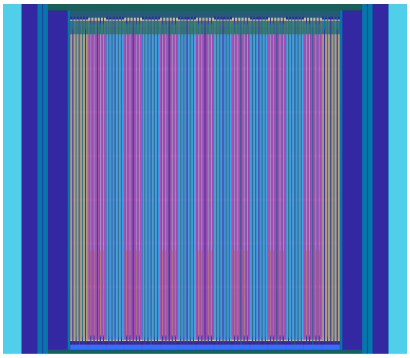
Problem 2

The lattice eigenvalues matched the reference solution well overall, with the greatest difference in any case being less than 80 pcm. The complete set of eigenvalues may be found in Table II.

Pin powers were also in agreement. Problem 2a, for example, had a maximum discrepancy of 0.52% (Fig. 5), while



(a) Radial



(b) Axial

Fig. 4: Full core

Problem 2k's maximum discrepancy was 0.43% from the reference solution (Fig. 6). Note that the reference, and therefore the plots, assume octant symmetry.

Problem 3

The eigenvalues for Problem 3 were within 50 pcm of their expected values: see Table III. A comparison of the axial power profiles revealed maximum relative differences of 0.83% and 1.01% at the bottom of the assembly for Cases 3a and 3b, respectively. Errors away from the edges were on the order of hundredths of a percent for both cases. The axial power profiles are shown in Fig. 7.

Full-core Problems

Numeric values for the power distribution in full-core cases were not included in the benchmark specification document due to their size. Notwithstanding, an eigenvalue calculation was still performed for Problem 5a-1, giving k_{eff}= 0.99991 $\pm$ 0.00001. This agrees within 1.1 pcm of the benchmark solution's value: 0.999899 $\pm$ 0.000010.

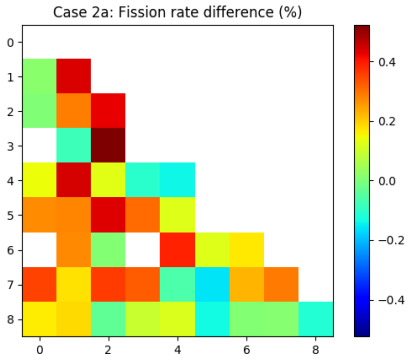


Fig. 5: Radial power profile comparison for Problem 2a.

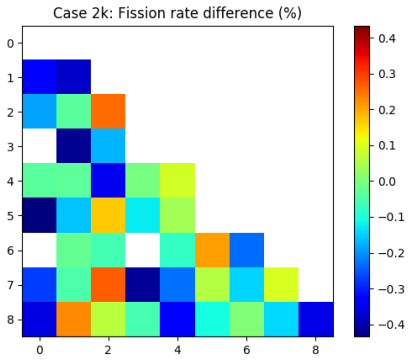


Fig. 6: Radial power profile comparison for Problem 2k.

CONCLUSIONS

We expected a certain degree of discrepancy between OpenMC and the reference solutions for VERA's benchmarks due to CASL's use of ENDF/B-VII.0 and our use of ENDF/B-VII.1. Nevertheless, all eigenvalue calculations were within 100 pcm of the expected results, the pin powers were within a fraction of a percent, and the axial power profile in Problem 3 matched satisfactorily. We conclude that Vera-to-OpenMC is capable of converting these models faithfully.

FUTURE WORK

Future work will involve obtaining the detailed reference solution for the full core cases and comparing the pin power distributions and eigenvalues between OpenMC and the benchmark for each.

Additionally, a more user-friendly interface for Vera-to-OpenMC is needed. This is an area of active development.

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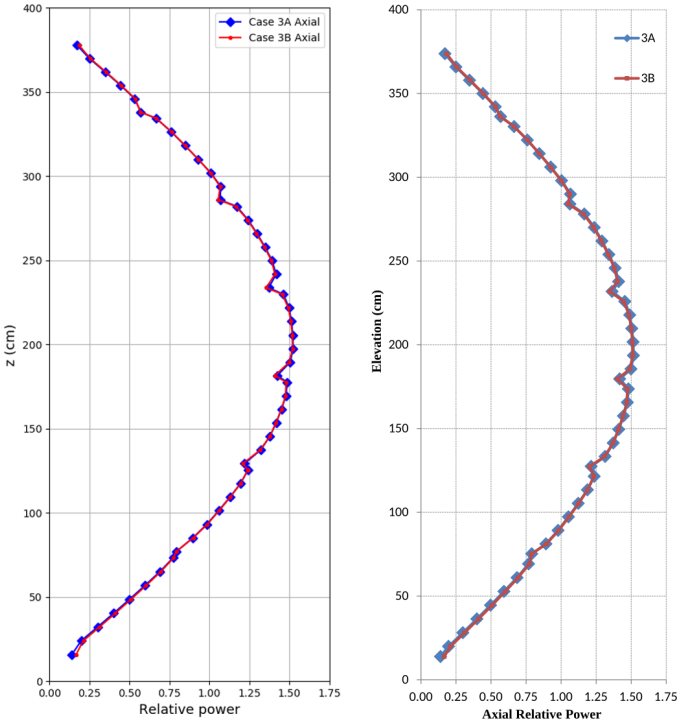

Fig. 7: The axial power profile from OpenMC (left) compared to that of VERA (right) for Problem 3.

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APPENDIX

TABLE I: Problem 1 – 2D Pincell Results

Case	Description	Fuel Temp. (K)	Moderator Density (g/cm^3)	k_{eff} – VERA ENDF/B-VII.0	k_{eff} – OpenMC ENDF/B-VII.1	Δk_{eff} (pcm)
1A	No poisons	600	0.743	1.187038 ± 0.000054	1.18496 ± 0.00014	20.7
1B	No poisons	600	0.661	1.182149 ± 0.000068	1.18183 ± 0.00014	20.8
1C	No poisons	900	0.661	1.171722 ± 0.000072	1.17155 ± 0.00015	22.2
1D	No poisons	1200	0.661	1.162603 ± 0.000071	1.16317 ± 0.00014	21.1
1E	IFBA	600	0.743	0.771691 ± 0.000076	0.77153 ± 0.00012	19.6

TABLE II: Problem 2 – 2D Lattice Results

Case	Description	Fuel Temp. (K)	Moderator Density (g/cm^3)	k_{eff} – VERA ENDF/B-VII.0	k_{eff} – OpenMC ENDF/B-VII.1	Δk_{eff} (pcm)
2A	No poisons	600	0.743	1.182175 ± 0.000017	1.18010 ± 0.00015	71.8
2B	No poisons	600	0.661	1.183360 ± 0.000024	1.18280 ± 0.00015	56
2C	No poisons	900	0.661	1.173751 ± 0.000023	1.17358 ± 0.00014	17.1
2D	No poisons	1200	0.661	1.165591 ± 0.000023	1.16586 ± 0.00014	26.9
2E	12 Pyrex	600	0.743	1.069627 ± 0.000024	1.06935 ± 0.00015	27.7
2F	12 Pyrex	600	0.743	0.976018 ± 0.000026	0.97547 ± 0.00014	54.8
2G	24 AlC	600	0.743	0.847695 ± 0.000025	0.84759 ± 0.00013	10.5
2H	24 B4C	600	0.743	0.788221 ± 0.000025	0.78745 ± 0.00012	77.1
2I	Instrument thimble	600	0.743	1.179916 ± 0.000024	1.17954 ± 0.00014	37.6
2J	24 Pyrex + Instrument thimble	600	0.743	0.975193 ± 0.000025	0.9748 ± 0.00014	39.3
2K	24 Pyrex + Radially zoned fuel	600	0.743	1.020063 ± 0.000025	1.02002 ± 0.00013	4.3
2L	80 IFBA	600	0.743	1.018915 ± 0.000024	1.01847 ± 0.00013	45
2M	128 IFBA	600	0.743	0.938796 ± 0.000025	0.93868 ± 0.00014	11.6
2N	104 IFBA + 20 WABA	600	0.743	0.869615 ± 0.000025	0.86897 ± 0.00005	65
2O	12 Gadolinia	600	0.743	1.047729 ± 0.000024	1.04762 ± 0.00013	10.9
2P	24 Gadolinia	600	0.743	0.927410 ± 0.000024	0.92733 ± 0.00013	8
2Q	Gridded	565	0.743	1.171940 ± 0.000016	1.17154 ± 0.00015	40

TABLE III: Problem 3 – 3D Assembly Results

Case	Description	Fuel Temp. (K)	Moderator Density (g/cm^3)	k_{eff} – VERA ENDF/B-VII.0	k_{eff} – OpenMC ENDF/B-VII.1	Δk_{eff} (pcm)
3A	No poisons	600	0.743	1.175722 ± 0.000005	1.17523 ± 0.00002	49.2
3B	24 Pyrex	565	0.743	1.000154 ± 0.000006	1.00014 ± 0.00001	1.4