VERA-to-OpenMC

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VERA

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]

Objectives

VERA comes with a detailed set of core physics benchmarks based on the initial core of Watts Bar Nuclear Plant, Unit 1 (WBN1).[3] Each benchmark problem is specified in a single ASCII input deck, which is used for all of VERA's physics codes. A Perl script in the VERA common input processor parses these input decks to XML files.

We wished to compare the criticality calculations from OpenMC and from VERA for each of the benchmark problems. A Python program, **VERA-to-OpenMC**, was written to take the processed XML files for each VERA input and use the Python API of OpenMC to construct the corresponding model.

Examples

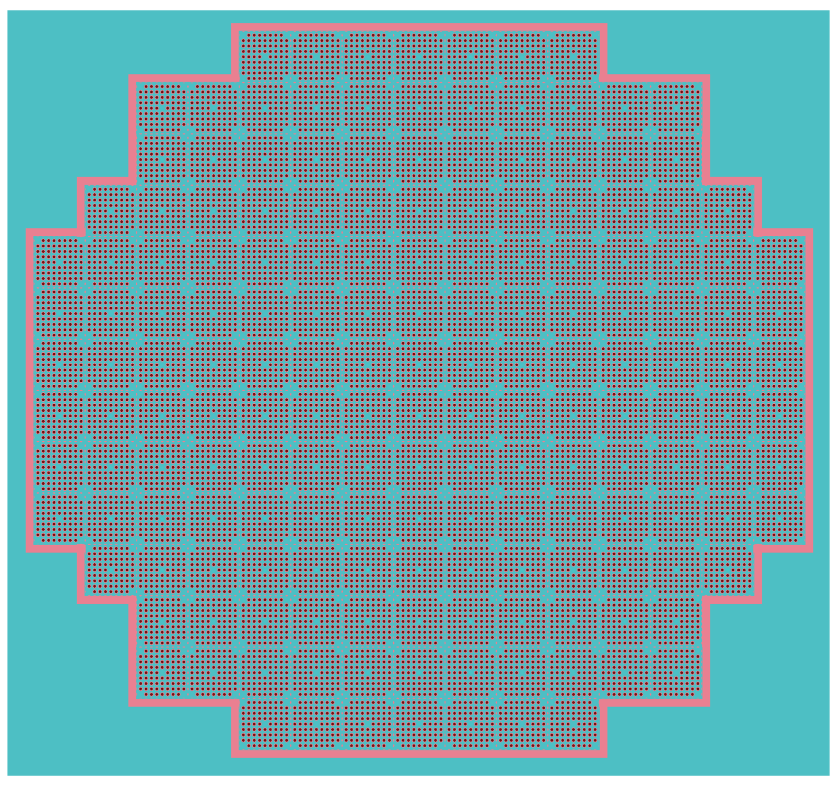

Figure 2. A core baffle. In its current state, VERA-to-OpenMC can add a baffle around the fuel for an abritrary core shape. Future work will include the core barrel, the neutron shields, and the reactor pressure vessel.

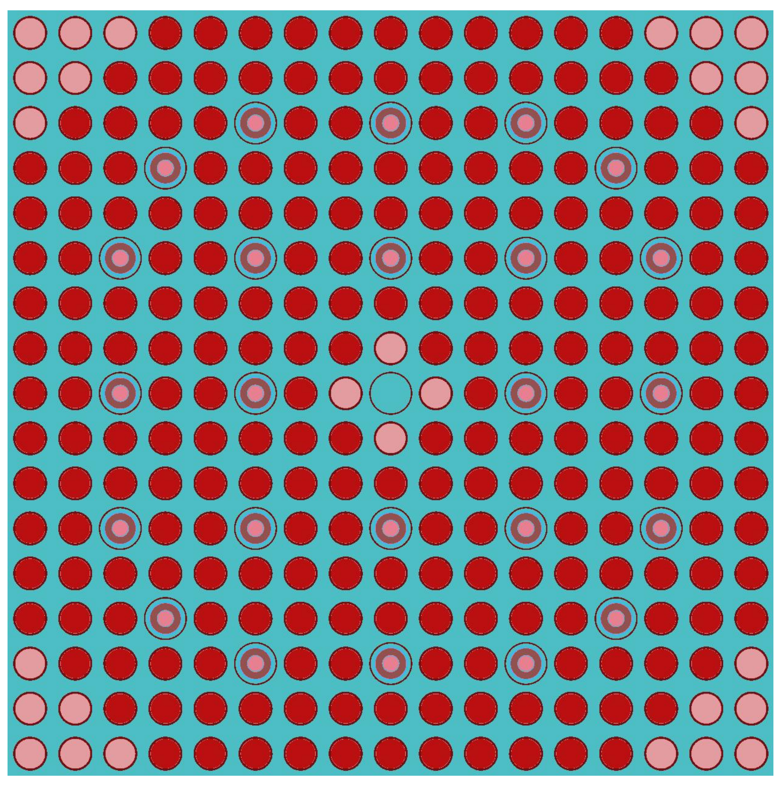

Figure 3. 17×17 fuel assembly lattice, as appears in Cases 2A-P. This particular lattice is from Case 2K, which features radially zoned fuel enrichments, 24 burnable poison insertions, and an empty guide tube for instrumentation.

Results

Case	Description	Fuel Temperature (K)	Moderator Density (g/cm³)	k_{eff} – VERA endfb7.0	k_{eff} – OpenMC endfb7.1	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 1. Results for Progression Problem 1:
Single Westinghouse fuel rod cell at beginning of life.

Case	Description	Fuel Temperature (K)	Moderator Density (g/cm³)	k_{eff} – VERA endfb7.0	k_{eff} – OpenMC endfb7.1	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	56.0
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 AIC	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	–	–
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	–	–
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	8.0

Table 2. Results for Progression Problem 2:
Single Westinghouse-type 17×17 fuel lattice at beginning of life.

OpenMC

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) converted to HDF5.

Methodology

VERA's input decks are concise, and much of the geometry is constructed "behind the scenes." Therefore, it was necessary to model a generic PWR geometry in OpenMC based on the core, assembly, and pin cell dimensions given in the decks. Some challenging components included:

- Core baffle
- Neutron pads
- Nozzles
- Grid spacers
- Core insertions (control rods, burnable poisons, and detectors)

The Python API of OpenMC was used to create the reactor model using constructive solid geometry. Due to the complexity of some of the geometries involved, only results from Problem 1 (pin cell cases – Table 1) and Problem 2 (17×17 Westinghouse-style fuel lattices – Table 2) are available at this time. However, the full-core converter is nearing completion.

For all criticality calculations, the following Monte Carlo simulation parameters were used:

- Number of inactive batches: 75
- Total number of batches: 275
- Particles per batch: 200,000

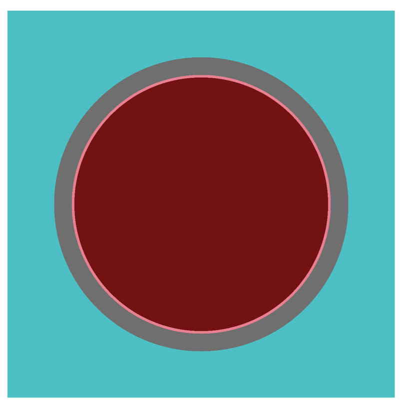

Figure 1. Single pin cell, as appears in Cases 1A-E

Cross Sections and 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 as provided with MCNP6. For thermal scattering, continuous-energy $S(\alpha, \beta)$ tables were used for hydrogen in the moderator.

Conclusions

We anticipated some discrepancy due to our use of ENDF/B-VII.1 cross sections, whereas CASL used ENDF/B-VII.0 for their solutions. All results were within 100 pcm, which seems reasonable given the differences between the data libraries. At this time, VERA-to-OpenMC fails to convert Cases 2L and 2N. We are currently investigating this bug.

Development of the full-core converter is still in progress. Further work is required to create the full 3-D fuel assemblies and to model the core barrel, neutron shields, and reactor vessel.

References and Acknowledgements

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Works Cited:

1) Scott Palmtag, Andrew Godfrey. "VERA Common Input User Manual." Consortium for Advanced Simulation of LWRs (2015). CASL-U-2014-0014-002
2) Paul K. Romano, Benoit Forget. The OpenMC Monte Carlo Particle Transport Code, Annals of Nuclear Energy, Volume 51, January 2013, Pages 274-281, ISSN 0306-4549, http://dx.doi.org/10.1016/j.anucene.2012.06.040.
3) Andrew T. Godfrey. "VERA Core Physics Benchmark Progression Problem Specifications." Consortium for Advanced Simulation of LWRs (2014). CASL-U-2012-0131-004