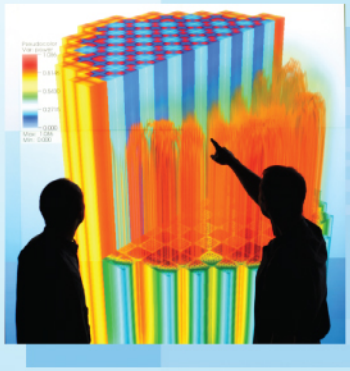
Power uprates
and plant life extension

CASL-U-2013-0284-000

Consortium for Advanced Simulation of LWRs



Engineering design
and analysis

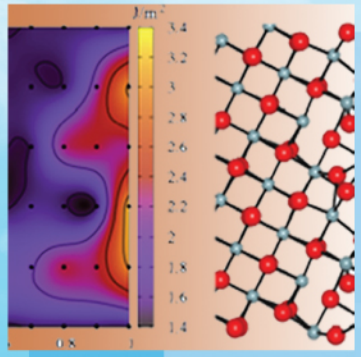
VERA Benchmark Calculations using the SCALE-Polaris Lattice Physics Code

Science-enabling
high performance
computing

M. A. Jessee, W. A. Wieselquist, M. L. Williams, K. S. Kim

Oak Ridge National Laboratory

November 10-14, 2013



Fundamental science

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

VERA Benchmark Calculations Using the SCALE-Polaris Lattice Physics Code

Matthew A. Jessee, William A. Wieselquist, Mark L. Williams, and Kang Seog Kim

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831 USA, jesseema@ornl.gov

INTRODUCTION

Polaris is a new in-development computational module within the SCALE code system [1] that provides 2-D lattice physics analysis capability for light water reactor (LWR) fuel designs. In this work, Polaris has been applied to a series of pin and lattice numerical benchmarks developed by and for the U.S. Department of Energy CASL Innovation Hub (Consortium of Advanced Simulation of Light Water Reactors). An overview of the Polaris methodology is provided, along with the results and analysis of the benchmark calculations.

SELF-SHIELDING METHODOLOGY

Polaris is a 2-D lattice physics code that utilizes a new multigroup self-shielding method called the Embedded Self-Shielding Method (ESSM) [2] and a new transport solver based on the Method-of-Characteristics (MoC). The ESSM approach computes multigroup self-shielded cross sections using Bondarenko interpolation. The background cross section utilized in the interpolation is determined by a series of 2-D MoC fixed source calculations, similar to the subgroup method. In contrast to the subgroup method, which requires fixed source calculations per subgroup level per energy group, ESSM requires only one fixed source calculation per energy group. However, the fixed source calculation must be solved in an iterative manner in which the cross sections depend on the fixed source flux distribution. If the number of iterations needed to update the cross sections in ESSM is less than the number of fixed source calculations utilized in the subgroup method, then the ESSM method is more computationally efficient. Additional details on ESSM are provided in Ref. 2.

Polaris currently employs ESSM with either a 252-group or a 56-group ENDF/B-VII-based library, generated by the AMPX code system [3]. The library contains cross sections, intermediate resonance (IR) parameters, and full-range Bondarenko factors for 422 nuclides. Bondarenko factors for U-235, U-238, Pu-239, Pu-240, and Pu-241 were generated based on heterogeneous equivalence theory, a procedure that ensures the ESSM calculation reproduces the self-shielded cross sections computed from a series of reference 2-D MoC continuous-energy unit cell calculations. The set of unit cell configurations was selected to span the range of self-shielding for these isotopes.

TRANSPORT METHODOLOGY

Polaris utilizes the self-shielded cross sections within a multigroup 2-D k-calculation using the new MoC transport solver. Various run-time speedups, including an intermediate group collapsing procedure and coarse-mesh finite difference (CMFD) acceleration, remain under investigation. The MoC solver has been developed within Denovo, which was originally developed for parallel 3-D Cartesian mesh multigroup discrete ordinates (S_N) calculations [4]. The Denovo framework has been designed such that both transport solver implementations (i.e., 3-D S_N, 2-D MoC) utilize the same iterative methods and parallel energy decomposition strategies. Polaris currently employs the biconjugate gradient stabilized (BiCGSTAB) method for the fast-range within-group calculations and for the thermal-range upscatter calculation, and power iteration for the eigenvalue calculation. Although Polaris currently utilizes a serial version of the Denovo MoC solver, energy parallelism is under investigation. By default, transport-corrected P_0 scattering is utilized for the k-calculation, but higher-order scattering options are available.

Polaris also provides a critical spectrum calculation for correcting the flux distribution for computing both few-group homogenized cross-section edits and depletion reaction rates. In the initial development, only pressurized water reactor (PWR) assembly geometries are supported. An example 17×17 PWR assembly model is shown in Fig. 1.

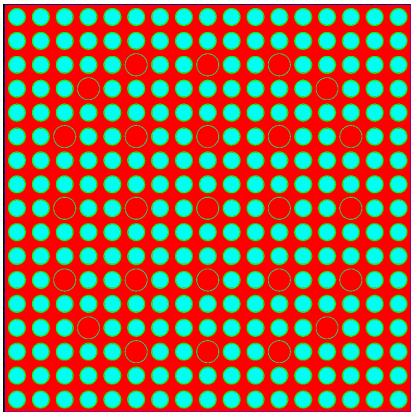


Fig. 1. 17×17 PWR assembly geometry in Polaris.

DEPLETION METHODOLOGY

Polaris is integrated with the SCALE/ORIGEN [5] depletion code for depletion calculations. The depletion of each pin—or radial subregion of the pin—is based on the local normalized flux distribution. Cross-section values in the ORIGEN transition matrix are updated from the multigroup self-shielded cross sections and the multigroup flux distribution for each depletion region. The critical-spectrum correction to the flux distribution for depletion is controlled by an input user option. The cross-section updates are performed in-memory as compared to the file-based approach utilized in the SCALE/TRITON lattice physics sequence [6].

BENCHMARK RESULTS

The VERA (Virtual Environment for Reactor Applications) benchmark progression problems have been established to measure progress and assess accuracy of emerging core simulation capabilities within the CASL Innovation Hub [7]. These calculational benchmarks are defined from actual fuel and plant data from the initial core loading of Watts Bar Unit 1, a PWR with Westinghouse 17×17 fuel assemblies.

Polaris calculations were performed using the 56-group library for the first and second problem sets of the VERA benchmark set. The first set contains five pin cell benchmarks, and the second set contains 16 lattice benchmarks. The full description for these benchmark problems is provided in Ref. 7. The problems have been developed for fresh UO_2 fuel (3.1 wt % U-235 enrichment) at the Hot-Zero-Power (HZP) beginning-of-cycle critical boron condition of ~1300 ppm boron. A brief description for each of the benchmark problems modeled in this work is provided in Table I. Unless otherwise stated in Table I, all material temperatures are modeled at 600 K, and the coolant density is modeled at 0.743 g/cm^3. All lattice calculations were performed using quarter-symmetry geometry.

Table II shows the Polaris k_{eff} values for the five pin cell benchmarks, compared to reference continuous energy (CE) KENO results from Ref. 7. Polaris exhibits a slight temperature bias in cases 1B through 1D, where the reactivity difference decreases as the fuel temperature increases. Investigations have shown that this bias can be minimized with an improved treatment for the temperature dependence of the removal cross section. In future development, an additional Bondarenko factor for the removal cross section will be introduced to the multigroup library and the scattering matrices will be renormalized to account for the self-shielding of the removal cross section.

Quadrature refinement investigations were performed to determine the appropriate MoC quadrature. For all cases, including the lattice benchmarks, a Tabuchi-Yamamoto (TY) [8] product quadrature set was used with three polar angles per octant and 20 azimuthal angles per octant. For cases 1A through 1D, the MoC ray spacing was 0.03 cm. For case 1E, 0.003 cm ray spacing was selected to appropriately model the thermal flux depression in the IFBA coating. An approach to reduce the ray spacing for IFBA problems, via homogenization or an alternative approach, remains under investigation. Transport-corrected P_0 scattering treatment was also utilized for the benchmark calculations.

The VERA lattice benchmark calculational results are shown in Table III. Both reactivity differences and pin-wise fission rate differences are provided. The CE-KENO-VI uncertainties are approximately 2×10^{-5} for k_{eff} and less than 0.06% for pin fission rates. The results exhibit a similar reactivity bias with temperature for cases 2B through 2D as 1B through 1D. The other cases show

TABLE I. VERA benchmark description

ID	Description
1A	565 K (pin cell)
1B	0.661 g/cm^3 coolant
1C	0.661 g/cm^3 coolant, 900 K fuel
1D	0.661 g/cm^3 coolant, 1200 K fuel
1E	0.001 cm IFBA[a] (ZrB_2)
2A	565 K (lattice)
2B	0.661 g/cm^3 coolant
2C	0.661 g/cm^3 coolant, 900 K fuel
2D	0.661 g/cm^3 coolant, 1200 K fuel
2E	12 Pyrex poison rods
2F	24 Pyrex poison rods
2G	24 AgInCd control rods
2H	24 B_4C control rods
2I	Instrument thimble
2J	Instrument thimble + 24 Pyrex
2K	Radially zoned enrichment + 24 Pyrex
2L	80 IFBA
2M	128 IFBA
2N	104 IFBA + 20 WABA[b]
2O	12 Gd_2O_3-integral burnable absorber rods
2P	24 Gd_2O_3-integral burnable absorber rods

[a]Integral fuel burnable absorber.
[b]Wet annular burnable absorber.

TABLE II. VERA pin cell benchmark results

ID	CE-KENO-VI k_{eff} (SD[a])	Polaris k_{eff}	Δρ (pcm)
1A	1.18782 (7)	1.18631	-107
1B	1.18294 (7)	1.18143	-108
1C	1.17239 (8)	1.16999	-174
1D	1.16315 (7)	1.16015	-222
1E	0.77237 (8)	0.77101	-228

[a]Standard deviation from CE-KENO-VI ($\times 10^5$).

TABLE III. VERA lattice benchmark results

ID	Δρ (pcm)	Pin power, % (RMS)	Pin power, % (max)
2A	-15	0.07%	0.21%
2B	-114	0.08%	0.19%
2C	-176	0.08%	0.15%
2D	-231	0.08%	0.17%
2E	-92	0.07%	0.18%
2F	-73	0.09%	0.21%
2G	-59	0.19%	0.37%
2H	203	0.17%	0.36%
2I	-121	0.08%	0.20%
2J	-66	0.09%	0.21%
2K	-72	0.10%	0.26%
2L	-167	0.11%	0.23%
2M	-194	0.12%	0.25%
2N	-176	0.12%	0.27%
2O	-85	0.11%	0.28%
2P	-36	0.14%	0.32%

good agreement for both k_{eff} and pin fission rates. The same quadrature sets were utilized for the lattice calculations as the pin-cell calculations, with an order-of-magnitude finer ray spacing for the IFBA cases (i.e., 2L, 2M, and 2N) than for non-IFBA cases. These calculations were performed on a Linux workstation using 2.6 GHz AMD Opteron™ processors. The average run-time for the non-IFBA cases was 5 minutes, although 2 minute run-times are achievable for a TY-quadrature set with 2 polar angles per octant, 16 azimuthal angles per octant, and 0.08 cm ray spacing. The coarser quadrature options produce a reactivity difference less than 15 pcm and negligible difference in pin powers compared to the quadrature options utilized for the benchmark calculations. The average run-time for the IFBA cases is currently 30 minutes due to the finer ray spacing that is currently required. The memory requirement for 56-group non-IFBA lattice calculations is ~500 megabytes.

CONCLUSIONS

A new 2-D LWR lattice physics capability, named Polaris, is being developed for the release of SCALE 6.2. In this work, the Polaris methodology has been introduced and calculation results provided for the CASL VERA pin and lattice benchmark sets. The results demonstrate that Polaris provides acceptable predictions for HZP PWR pin and lattice calculations at beginning of life by comparison to CE-KENO-VI. A bias in k_{eff} as a function of fuel temperature has been identified, and can be reduced by modifications to the removal cross-section methodology. Code development efforts to reduce computational run-time are under investigation, which include the implementation of CMFD, diagonal symmetry, and an intermediate energy group collapsing procedure.

ACKNOWLEDGMENTS

The authors would like to thank the U.S. Nuclear Regulatory Commission for the development of Polaris.

Notice: This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

REFERENCES

1. *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1, June 2011. (Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.)
2. M. WILLIAMS, K. KIM, "The Embedded Self-Shielding Method," PHYSOR 2012, Knoxville, Tennessee, USA, April 15-20, 2012.
3. M. DUNN, N. GREENE, "AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications," *Trans. Am. Nucl. Soc.* **86**, 118-119 (2002).
4. T. EVANS, A. STAFFORD, R. SLAYBAUGH, K. CLARNO, "DENOVO: A new three-dimensional parallel discrete ordinates code in SCALE," *Nucl. Technol.* **171**, 171-200 (2010).
5. I. GAULD et al., "Isotopic Depletion and Decay Methods and Analysis Capabilities in SCALE," *Nucl. Technol.* **174**(2), 169 (2011).
6. M. DEHART, S. BOWMAN, "Reactor Physics Methods and Analysis Capabilities in SCALE," *Nucl. Technol.* **174**(2), 196 (2011).
7. A. GODFREY, "VERA Core Physics Benchmark Progression Problem Specifications," CASL-U-2012-0131-002, http://www.casl.gov/publications.shtml (2013).
8. A. YAMAMOTO et al., "Derivation of Optimum Polar Angle Quadrature Set for the Method of Characteristics Based on Approximation Error for the Bickley Function," *J. Nucl. Sci. Technol.* **44**(2), 129 (2007).