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VERA Enhancements for Cross Section Shielding and Geometry Capabilities

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1. CROSS SECTION SHIELDING DEVELOPMENT

Two tasks were undertaken in FY22 that focus on VERA enhancements. The first task involved improvements to the new cross section shielding capability that was added to VERA in FY21. This cell-based capability solves the slowing down problem for each pin cell using Dancoff factors calculated from the whole-core problem. The Dancoff factors are determined for each subgroup level for important sets of materials such as fuel rods, control rods, fuel rods loaded with gad, etc. The cross section shielding is then performed for each cell using a 1D cylindrical collision probabilities (CP) calculation to obtain the equivalence cross sections required for the core transport calculations. The advantage of this method over the whole-core subgroup calculations is efficiency, since far fewer sweeps of the entire core are required.

FY22 work on cross section shielding focused on two tasks. First, work was done to extend this method to other reactors and components. The initial implementation focused only on pressurized water reactors (PWRs) with support for fuel rods, guide tubes, and control rods. To support boiling water reactors (BWRs), it was necessary to extend the capability to channel boxes and control blades. Both of these components can be accurately resolved using a one-group subgroup calculation (as was done for guide tubes in PWRs). The primary addition needed for BWRs was a second one-group subgroup calculation for hafnium, as some BWR control blades have hafnium tips. In addition to BWR support, support for fuel rods with gadolinium and burnable poison inserts was also added for PWRs.

A suite of 2D BWR problems comprising 30 BWR lattices with varying void, control blades, and other features was tested. The average keff difference between whole-core subgroup calculation and the new cell-based calculation was about 30 pcm, and the average pin power difference was about 0.04%, with a maximum of 0.33% for any case. A set of 20 3D BWR lattices was also run, with an average keff difference of 41 pcm, an average pin power difference of 0.32%, and a maximum pin power difference of 1.27%. The larger errors are expected for 3D BWR calculations given the presence of control blades and voiding. Additionally, it was found that the addition of the hafnium one-group calculation also caused minor improvements to the PWR calculations since the zircaloy cladding has trace amounts of hafnium.

The second task for FY22 was optimization of the cell-based shielding calculations. Several optimizations were attempted, with mixed results. The following optimizations were attempted and discarded:

- Modifications to the CP calculation to prevent duplicate computations
- Modifications to the branching structure in the function used to calculate the third-order Bickley–Naylor function
- Using single precision instead of double precision for the CP calculations
- Loosening solver tolerances for the CP calculations
- Link-time optimization (LTO).

LTO is unique in that it did effect a substantial improvement on the runtime, but it also caused unacceptably large solution changes and numerous test failures. Therefore, it was discarded until these errors can be further understood.

Two optimizations had positive impacts and were merged to the production branch. The first was the use of a multigroup transport sweep instead of a collection of one-group sweeps. There are approximately 10 sweeps required: one for each of the 4 subgroup levels for zirconium and hafnium, and one for the Dancoff factors for fuel rods, guide tubes, control rods, inserts, and fuel rods with gad. Performing all these sweeps together in one multigroup sweep with no scattering was found to be about 2.67 times as fast as using a one-group transport sweep. The second optimization was the use of function look-up tables for the Bickley–Naylor function evaluation. This replaced an old function that used piecewise polynomials and a large branching structure to evaluate the function. This resulted in an additional 15% speedup for large problems. Together, these two optimizations reduced a PWR cycle depletion runtime from 21 hours 31 minutes to 19 hours 42 minutes.

The cell-based shielding improvements are an important step toward achieving accuracy and performance improvements for light-water reactor (LWR) analysis support. In FY23, this cell-based shielding capability will be further improved using a “pin census” to further reduce the number of computations required without sacrificing accuracy. Then, on-the-fly cross section collapse will be implemented. This will allow LWR analysis using fewer energy groups that are collapsed with the proper energy spectrum for the calculation of interest. This will have a significant impact on the ability of the analyst to conduct long-running transient calculations or large sets of cycle depletions to analyze high-burnup or accident-tolerant fuels.

2. GEOMETRY CAPABILITIES

An additional FY22 task was the continued development of geometry capabilities and integration of those capabilities with VERA multiphysics coupling, with a focus on adding support for BWR modeling. These capabilities are being accomplished using Titan, the new geometry engine for VERA that allows modeling of complex geometries and will be used for modeling higher-fidelity BWR problems.

Figure 1 shows Titan’s capability to model complex BWR components such as channel boxes with rounded corners and indented/extruded edges, as well as cruciform-shaped control blades with horizontal holes drilled for absorber material. Once the geometry is built, Titan can either run Shift, or raytrace the geometry using utilities in SCALE for method-of-characteristics calculations.

Titan is currently under review by the SCALE team, and once in SCALE, it will provide a shared geometry engine for Shift and MPACT that allows for seamless code-to-code verification.

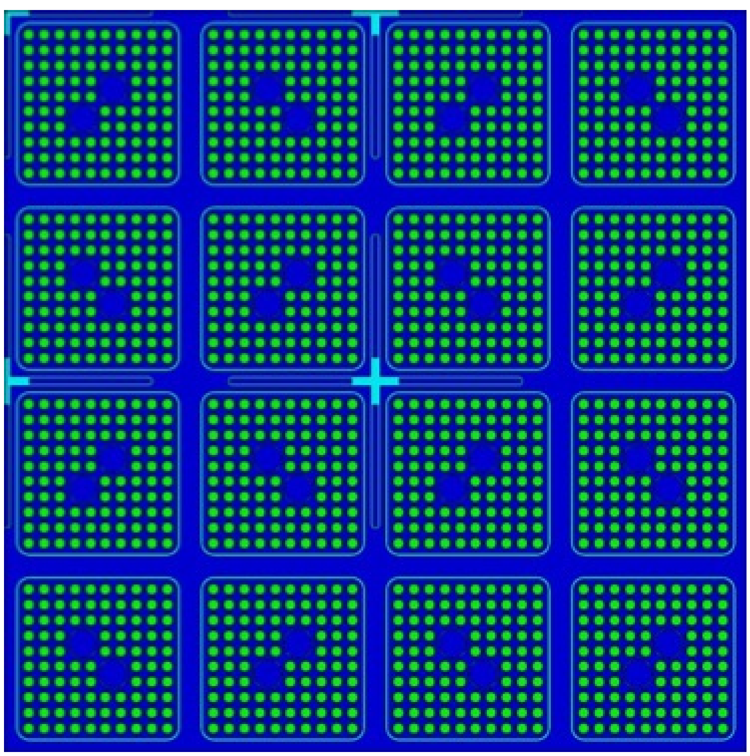

Figure 1: A higher-fidelity BWR core modeled with Titan.