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SIMPLIFICATION OF MULTIGROUP CROSS-SECTION PROCESSING FOR LARGE DEPLETION CALCULATIONS IN TRITON

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ABSTRACT

TRITON is the primary lattice physics module of the SCALE code system. Initially developed under U.S. Nuclear Regulatory Commission funding for high-fidelity mixed-oxide fuel assembly analysis, TRITON is now being used internationally for a wide variety of applications. However, for large heterogeneous lattice configurations, the cross-section processing required to obtain appropriately weighted burnup-dependent cross sections can be a bottleneck in a calculation. To overcome this issue, two new approaches have been implemented to simplify the cross-section processing requirements for lattice depletion calculations in TRITON. Both approaches were implemented and tested within TRITON and found to result in very little loss of accuracy in the rigorous multigroup cross-section weighting available within SCALE. Results of an analysis of a 9 × 9 boiling-water-reactor lattice in which 41 independent depletion pin cells were tracked are presented. These results show that the simplified cross-section processing option in TRITON results in a substantial reduction in computational time with very little loss of accuracy. The capabilities described herein are available within the latest update to the Version 5.1 release of SCALE.

Key Words: TRITON, NEWT, lattice physics

1. INTRODUCTION

The T-DEPL sequence of the TRITON module [1] within the SCALE code system [2] provides the ability to perform two-dimensional (2-D) lattice calculations to obtain cross sections and other lattice data for use in subsequent core simulator calculations [3]. TRITON provides automated, problem-dependent cross-section processing followed by calculation of the neutron multiplication factor for a 2-D system using the transport solver NEWT. This functionality can be iterated in tandem with ORIGEN-S depletion calculations to predict isotopic concentrations, source terms, and decay heat as a result of time-varying fluxes calculated in a 2-D deterministic fashion. TRITON has been developed in part to support lattice physics calculations through cross-section homogenization and group collapse, with branch state capabilities.

In calculations for large, heterogeneous fuel assemblies, it is often necessary to individually track nuclide inventories in each fuel pin; in addition, for strong poisons, the modeling of the pin should be sufficiently detailed (i.e., pin divided in rings) to capture radial burnup effects. Although symmetry can often be used to reduce the number of pins tracked, this number can still

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remain substantial, on the order of 20–30 pins. The SCALE system provides a rigorous mechanism for multigroup cross-section processing using the continuous-energy solver CENTRM [4] for self-shielding in the resolved resonance energy range, though this rigor has associated with it a computational cost. Generally, this computational burden is not significant for fresh fuel assemblies where no more than a handful of cells need be processed; however, the time required to process the multigroup cross sections for a large number of cells will often exceed the time required for the transport calculation itself. Additionally, the process of creating appropriately weighted multigroup cross sections using the continuous-energy spectrum obtained with CENTRM can be computationally expensive for depletion calculations for which hundreds of nuclides are contained in the transport model. This process is performed by the PMC module.

This paper describes two new approaches developed for TRITON to reduce the computational burden associated with multigroup cross-section processing and greatly accelerate the process with little impact on accuracy.

2. APPROACH

Two independent techniques were developed to reduce the computational burden associated with cross-section processing within TRITON. The first approach assumes that the microscopic cross sections are not significantly sensitive to the differences in nuclide number densities that occur during the depletion of fuel rods with initially identical compositions, even though nuclide number densities and hence macroscopic cross sections are known to diverge with burnup. The second approach recognizes that many fission product nuclides that build up during depletion are effectively infinitely dilute and may be treated as such during cross-section processing operations. The former approach reduces the number of pin cells that must be processed at each depletion step; the latter reduces the number of nuclides that must be spectrum weighted within each depleted pin cell. The following subsections describe each of these two approaches.

2.1. Cross-Section Processing for Similar Fuel Rods

In depletion calculations, multigroup cross sections change with the depletion of the initial fuel and the buildup of higher actinides and fission products. The depletion approach in TRITON ensures that the cross sections are updated with burnup in order to capture the effect of changing nuclide inventories as nuclear fuel is burned. Because the macroscopic cross sections used in transport and depletion calculations are more sensitive to nuclide number densities than they are to the microscopic cross sections of the nuclides themselves, it was hypothesized that for *similar* fuel rods, cross-section resonance processing could be simplified by performing calculations based on the average isotopic composition of rods in a set of similar rods. The definition of a set of *similar* rods remained to be determined, but as a first guess it was assumed that rods of the same initial enrichment would be similar over the life of an assembly.

To put this hypothesis to a test, the T-DEPL sequence in TRITON was modified to separate the cross-section processing functionality from the transport/depletion calculations. The ability was added to *assign* a set of mixtures in the transport and depletion phases to a single representative mixture for cross-section processing. The calculational procedure is illustrated in Fig. 1. In effect, the code is used to process cross sections for a set of *representative* mixtures.

Cross sections for these mixtures are duplicated for each *assigned* mixture. Transport and depletion calculations treat each mixture as distinct. At the end of each set of depletion calculations, the number densities for each set of assigned mixtures are averaged to update the number densities for the reduced set of representative mixtures. This process is repeated as TRITON performs periodic cross-section updates during a depletion calculation.

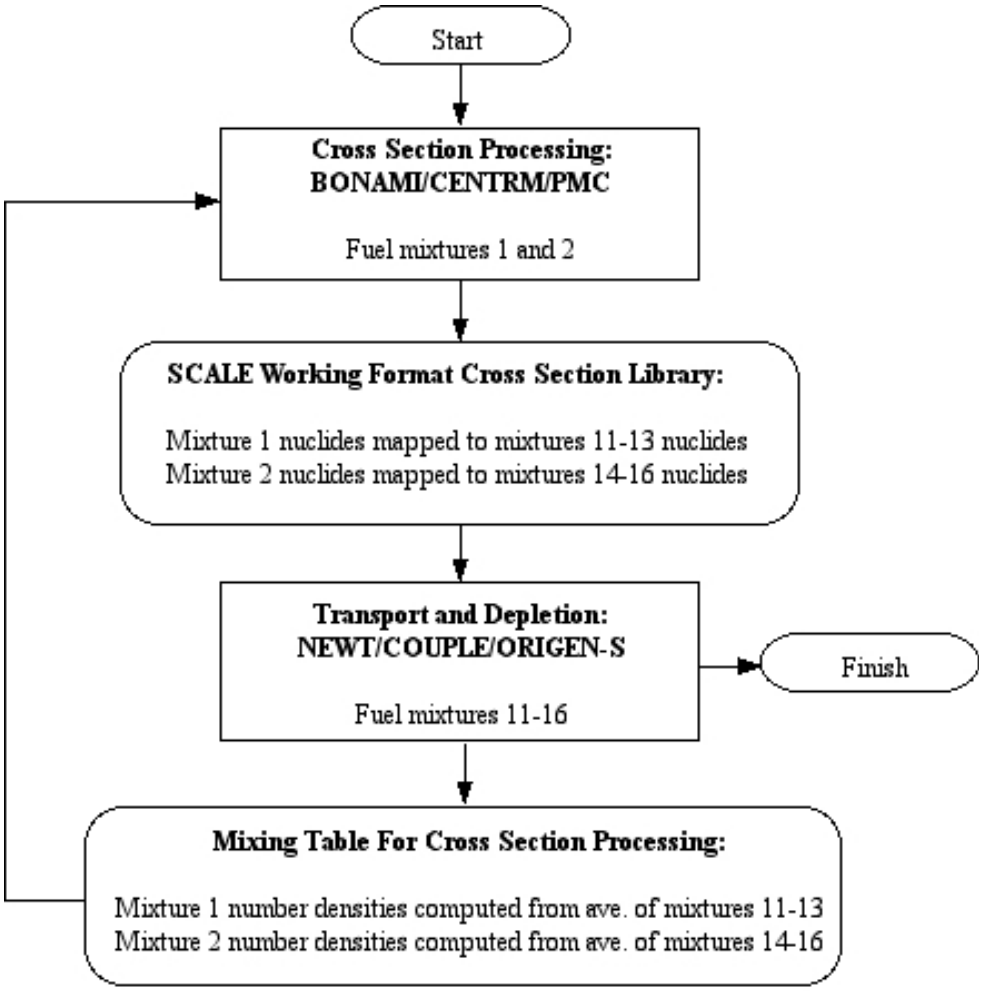

Figure 1. Schematic illustration of TRITON cross-section processing for similar fuel rods.

2.2. Infinite-Dilution Treatment for Low-Density Fission Products

The CENTRM module used for cross-section processing within SCALE performs an ultra-fine energy grid transport calculation using ENDF-based point data to generate an effectively continuous-energy neutron flux solution in the resonance energy range. This continuous-energy neutron flux is utilized in the PMC module to appropriately weight the multigroup cross sections to be used in subsequent transport calculations. The number of nuclides carried through a transport solution and used to update ORIGEN-S cross sections is defined by the user. Hundreds of fission product nuclides must usually be included in the transport calculation in order to accurately predict the system eigenvalue near end of life. Individually, most nuclides have very

little reactivity worth; however, taken as a whole, 200+ fission products can have a significant impact on reactivity.

TRITON has been updated to allow specification of a density cutoff, below which nuclides are not resonance weighted by PMC. This cutoff is defined as the ratio of a nuclide concentration to that of the largest nuclide concentration within a mixture, rather than as an absolute number density. The cutoff may be user defined; the default value is 10^{-8}. Early in the depletion simulation, there are only a handful of actinides and fission products for which the cross-section weighting by PMC is applicable; as fission product inventories increase and the relative number densities increase above the set threshold, the number of nuclides for which the weighting is carried out increases significantly.

This change in PMC processing will only affect the computational effort due to this change in PMC calculations; hence, the reduction of the total computational effort in the cross-section processing procedure will be small relative to the reduction due to the cross-section processing algorithm described earlier. However, this approach also significantly reduces the memory requirements of the code and permits calculations with hundreds of nuclides on machines that formerly would suffer from memory limitations within PMC.

3. RESULTS

To test the accuracy and performance gain for these two approaches, a depletion calculation was set up based on the Next-Generation Fuels benchmark specification [5] for a conceptual UO_2-fueled 9 × 9 boiling water reactor (BWR) design (Fig. 2). The fuel lattice is comprised of 74 fuel rods having five fuel enrichment values and includes 12 gadolinium-bearing rods. Using symmetry, this configuration can be reduced to include 41 independent fuel rods. However, because of the need to deplete gadolinium rods in rings, a total of 73 independently depleted mixtures are modeled, using five concentric rings of fuel in each of the six independent poison rod positions.

Multiple TRITON depletion models were developed; the first model used the standard approach in TRITON, in which pin cell calculations are performed for each of the 41 unique pin locations; this first case constitutes the referenced case. In the second model, cell processing was performed for only five pin cells, corresponding to five sets of similar fuel rods and representing the 41 unique fuel rod designs present, but the PMC infinite-dilution cutoff was set to zero, such that all nuclides were weighted using PMC. Finally, a set of calculations were performed with the reduced pin-cell processing approach, but with default cutoff values of 10^{-8}, 10^{-5}, 10^{-4}, and 10^{-3}. All models performed transport and depletion calculations for all 73 independent mixtures and included 232 actinides and fission products in the cross-section processing and transport calculations.

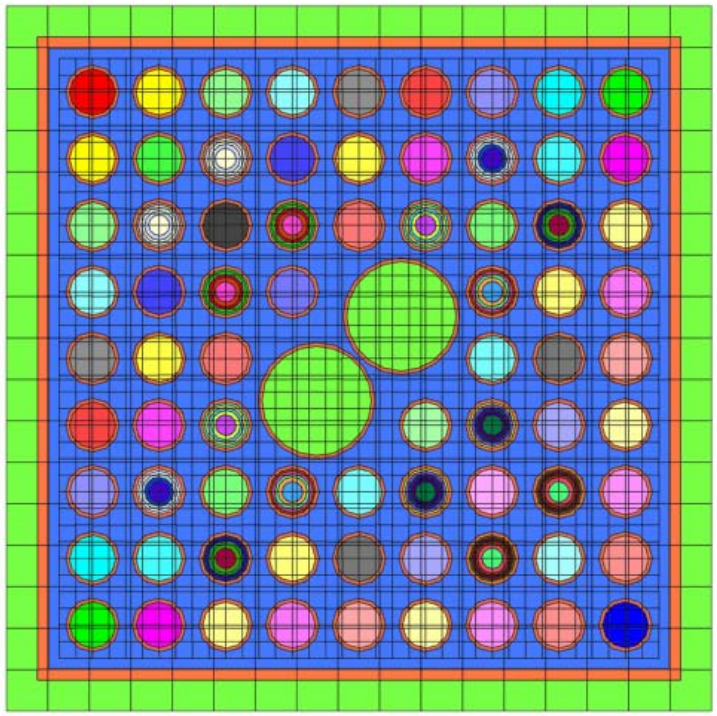

Figure 2. NEWT model for 9 × 9 BWR depletion calculation.

Figure 3 shows k_{eff} calculated as a function of burnup for all six models considered. With the exception of the low-resolution case that used a 10^{-3} cutoff value for resonance processing, the results are indistinguishable. Clearly, this cutoff value has reached a point where significant resonance effects are being ignored; nuclides omitted at this cutoff value are not well approximated as infinitely dilute. However, because the differences between the other solutions cannot be seen in this figure, Fig. 4 was produced to illustrate the percentage difference between the standard approach, representing a reference solution, and each of the approximating approaches (except the 10^{-3} cutoff case). The magnitude of the difference relative to the reference k_{eff} values remains below 0.1% over the entire period of time considered, with error increasing and peaking (and changing signs) as the gadolinium presented in the poison rods is depleted. Cases with a cutoff value of 10^{-5} or less have a maximum error of less than 0.02%. After full depletion of gadolinium, the difference between the methods decreases to effectively zero; late in life the error becomes larger than zero for all cases, indicating a very small bias in the cross-section assignment approximation.

Comparisons of predicted nuclide number densities show the same trends and errors of the same magnitude; results for a selected set of actinides and fission products are shown for all cases in Table I. Not surprisingly, the use of a 10^{-3} cutoff results in significant error in isotopic inventory predictions. The other cases show very good agreement. Results clearly indicate that use of the cross-section assignment technique and an infinite-dilution treatment for a concentration cutoff of 10^{-8} results in no significant loss of accuracy in inventory predictions. However, the computational time for each of the computational simplifications is significant. Table II

illustrates the time required to complete each model using SCALE running under Linux using a 2-GHz AMD Opteron 246 processor. The use of cross-section assignments reduced the computational effort by an order of magnitude. Small gains are seen in the use of the infinite-dilution cutoff. Interestingly, the largest cutoff value resulted in the greatest reduction in PMC processing time but required more computational time in the transport solution and a greater net run time.

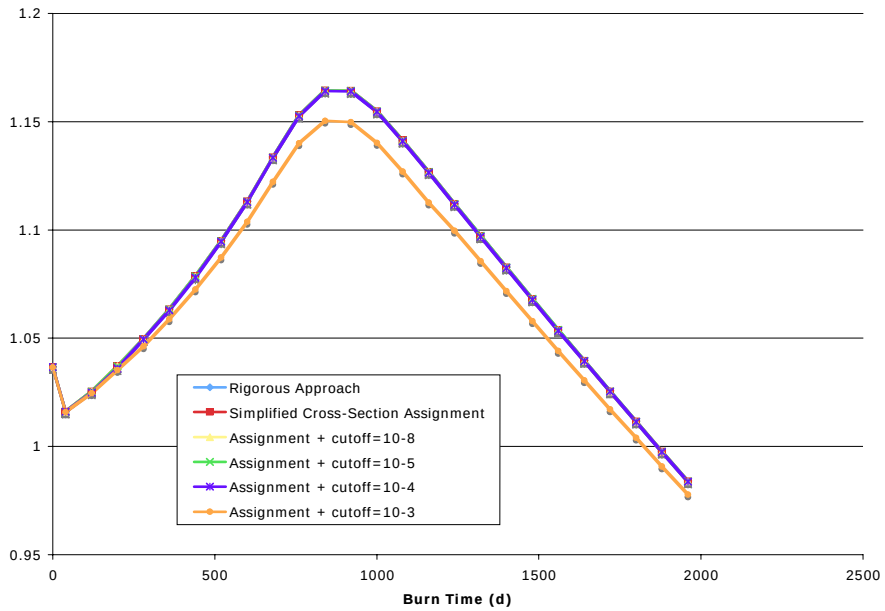

Figure 3. Results of BWR depletion calculations.

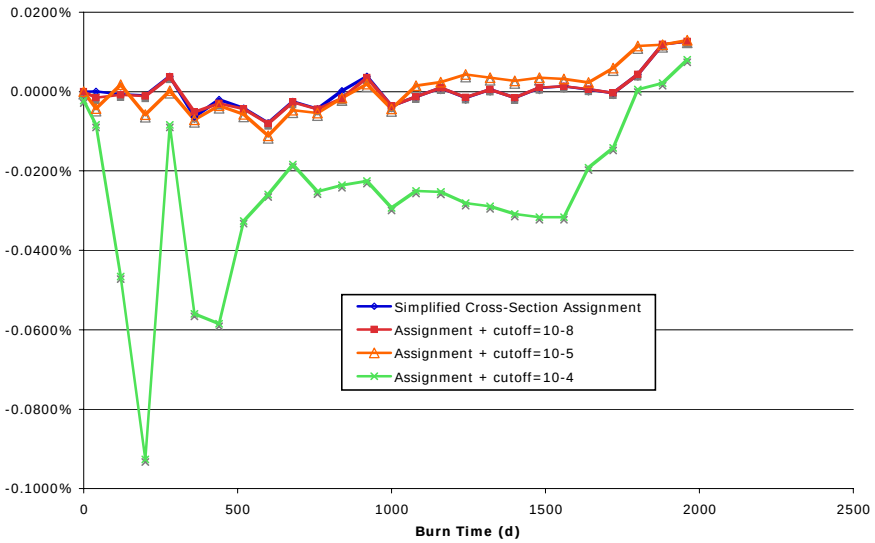

Figure 4. Error relative to reference case for BWR depletion calculations.

Table I. Predicted end-of-life nuclide number densities under various approximations

	Rigorous standard approach	Assignment cutoff = 0	Assignment + 10^{-8} cutoff	Assignment + 10^{-5} cutoff	Assignment + 10^{-4} cutoff	Assignment + 10^{-3} cutoff
^{234}U	1.09E–07	1.09E–07	1.09E–07	1.11E–07	1.11E–07	1.12E–07
^{235}U	3.26E–04	3.26E–04	3.26E–04	3.26E–04	3.26E–04	3.35E–04
^{236}U	1.50E–04	1.50E–04	1.50E–04	1.50E–04	1.50E–04	1.49E–04
^{238}U	2.02E–02	2.02E–02	2.02E–02	2.02E–02	2.02E–02	2.02E–02
^{238}Pu	6.01E–06	6.01E–06	6.01E–06	6.01E–06	6.00E–06	6.06E–06
^{239}Pu	1.22E–04	1.22E–04	1.22E–04	1.22E–04	1.22E–04	1.26E–04
^{240}Pu	5.96E–05	5.96E–05	5.96E–05	5.96E–05	5.96E–05	3.95E–05
^{241}Pu	3.11E–05	3.11E–05	3.11E–05	3.11E–05	3.11E–05	3.65E–05
^{242}Pu	1.47E–05	1.47E–05	1.47E–05	1.47E–05	1.47E–05	1.67E–05
^{243}Pu	2.56E–09	2.56E–09	2.56E–09	2.56E–09	2.56E–09	3.27E–09
^{241}Am	1.72E–06	1.72E–06	1.72E–06	1.72E–06	1.72E–06	2.13E–06
^{242m}Am	3.56E–08	3.55E–08	3.55E–08	3.55E–08	3.56E–08	4.37E–08
^{243}Am	3.62E–06	3.62E–06	3.62E–06	3.63E–06	3.68E–06	4.83E–06
^{242}Cm	4.19E–07	4.19E–07	4.19E–07	4.18E–07	4.19E–07	4.94E–07
^{243}Cm	1.20E–08	1.20E–08	1.20E–08	1.28E–08	1.29E–08	1.55E–08
^{244}Cm	1.31E–06	1.31E–06	1.31E–06	1.31E–06	1.28E–06	1.46E–06
^{245}Cm	7.23E–08	7.25E–08	7.25E–08	7.16E–08	6.09E–08	7.04E–08
^{95}Mo	5.94E–05	5.94E–05	5.94E–05	5.94E–05	5.94E–05	5.90E–05
^{99}Tc	6.45E–05	6.45E–05	6.45E–05	6.45E–05	6.45E–05	6.40E–05
^{101}Ru	6.08E–05	6.08E–05	6.08E–05	6.08E–05	6.08E–05	6.08E–05
^{103}Rh	3.14E–05	3.14E–05	3.14E–05	3.14E–05	3.14E–05	3.26E–05
^{109}Ag	4.66E–06	4.66E–06	4.66E–06	4.66E–06	4.70E–06	4.89E–06
^{133}Cs	6.67E–05	6.67E–05	6.67E–05	6.67E–05	6.67E–05	6.66E–05
^{143}Nd	4.32E–05	4.32E–05	4.32E–05	4.32E–05	4.32E–05	4.35E–05
^{145}Nd	3.70E–05	3.70E–05	3.70E–05	3.70E–05	3.70E–05	3.66E–05
^{147}Sm	6.20E–06	6.20E–06	6.20E–06	6.20E–06	6.11E–06	5.78E–06
^{149}Sm	9.02E–08	9.02E–08	9.02E–08	9.03E–08	9.03E–08	9.74E–08
^{150}Sm	1.50E–05	1.50E–05	1.50E–05	1.50E–05	1.50E–05	1.45E–05
^{151}Sm	6.14E–07	6.14E–07	6.14E–07	6.13E–07	6.02E–07	7.23E–07
^{152}Sm	4.89E–06	4.89E–06	4.89E–06	4.89E–06	5.00E–06	5.47E–06
^{153}Eu	6.02E–06	6.02E–06	6.02E–06	6.02E–06	5.93E–06	6.04E–06
^{155}Gd	4.57E–08	4.57E–08	4.57E–08	4.56E–08	4.58E–08	5.06E–08

Table II. Calculational time required for various modeling approaches

Model	Time (hours)
Rigorous (reference) approach	117.62
Simplified cross-section assignment	12.08
Assignment + 10^{-8} cutoff	11.74
Assignment + 10^{-5} cutoff	11.48
Assignment + 10^{-4} cutoff	11.32
Assignment + 10^{-3} cutoff	12.04

4. CONCLUSIONS

The results provided here clearly demonstrate that the two simplifying approaches for cross-section processing recently implemented in the TRITON module within SCALE 5.1 provide substantial benefit in terms of computational requirements without a significant reduction in accuracy (unless an inappropriately large cutoff value is used). This is a first phase of ongoing research at the Oak Ridge National Laboratory in methods development to improve performance of TRITON for large-scale depletion analysis, so that the high-fidelity resolution of TRITON calculations can be used for detailed lattice calculations in a computationally efficient manner.

Note that the ability to perform reduced cell calculations using cross-section assignment within TRITON was made available in the Version 5.1 release of SCALE. The number density cutoff for infinite-dilution treatment was completed after the initial release, but this version of TRITON is available for download from the SCALE web site, http://www.ornl.gov/sci/scale, for users who have a registered version of SCALE 5.1.

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