SCALE 5: Powerful New Criticality Safety Analysis Tools

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Version 5 of the SCALE computer software system developed at Oak Ridge National Laboratory, scheduled for release in December 2003, contains several significant new modules and sequences for criticality safety analysis and marks the most important update to SCALE in more than a decade. This paper highlights the capabilities of these new modules and sequences, including continuous energy flux spectra for processing multigroup problem-dependent cross sections; one- and three-dimensional sensitivity and uncertainty analyses for criticality safety evaluations; two-dimensional flexible mesh discrete ordinates code; automated burnup-credit analysis sequence; and one-dimensional material distribution optimization for criticality safety.

KEYWORDS: SCALE, TSUNAMI, SMORES, Javapeno, STARBUCS, NEWT, TRITON, CENTRM, KENO, sensitivity, uncertainty, optimization, burnup credit

1. Introduction

The SCALE (**S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuation)[1] computer software system developed at Oak Ridge National Laboratory (ORNL) is widely used and accepted around the world for criticality safety analyses. Version 5 of SCALE, scheduled for release in December 2003, contains several significant new modules and sequences for criticality safety analysis and marks the most important update to SCALE in more than a decade. This paper highlights the improvements to existing SCALE modules and the capabilities of new modules and sequences.

2. Improvements to Existing SCALE Modules

The following sections describe enhancements in SCALE 5 to currently existing SCALE modules.

2.1 Cross-Section Processing Enhancements

The cross-section processing capabilities in SCALE 5 have been expanded over the capabilities currently in SCALE 4.4a. Currently in SCALE 4.4a, only one unit cell can be specified and all other materials are treated as an infinite homogeneous medium. Resonance data must be manually added to the MORE DATA block to account for the geometry and lattice effects of materials not specified in the unit cell. In SCALE 5, the user may specify multiple unit cells. Each unit cell specification contains the cell type (infinite homogeneous medium, multiregion, or lattice cell), cell geometry type, and appropriate material and geometry data. Any number of unit cells may be specified, but each material may appear in only one unit cell. All materials not specified in a unit cell are processed as infinite homogeneous media.

NITAWL-III, an upgrade of NITAWL-II, has the capability to process multipole data, thus enabling it to process an ENDF/B-VI cross-section library with the Reich-Moore resonance parameters converted to multipole parameters. NITAWL uses the Nordheim Integral Treatment to process cross-section data in the resolved resonance range. Each resonance is processed individually, not accounting for the change in the background cross section due to other overlapping resonances. Also, a flux spectrum in the fuel lump is calculated based on the moderators and absorbers in the fuel lump and assuming a 1/E flux spectrum outside the lump as well as the slowing-down source above each resonance.

2.2 KENO V.a / KENO-VI

The KENO V.a and KENO-VI Monte Carlo criticality safety codes have been extensively modified for SCALE 5. Most of these modifications are transparent to the user. First, the codes have been completely rewritten in Fortran90. The large array that previously contained the cross-section and geometry data has been eliminated. In SCALE 5 the memory needed to store data in arrays is allocated dynamically as needed and deallocated when no longer needed. This greatly simplifies the overall program logic and removes the need for supergrouping. As a result, the supergrouping option has been eliminated.

A new algorithm is now used to determine the standard deviation associated with the system k_{eff} based on work by Ueki et al.[2] This algorithm accounts for the serial correlation between successive

generations, thus producing a more realistic standard deviation.

The codes now calculate a system mean-free path. This is done by first calculating a mean-free path for each generation. An average mean-free path over all generations and its standard deviation are then calculated. Region mean-free paths can also be calculated using the region macroscopic total cross section and the region fluxes.

The criticality search capabilities in SCALE 5 have been expanded to allow each unit cell to be explicitly identified with either a unit or a material that is being modified in KENO V.a. A search case may alter the material densities, the pitch of the cells in a lattice, or simple geometry boundaries. Since multiple unit cells are now allowed, a critical search may now be performed on lattices containing more than one fuel pin type. As the geometry or material in KENO V.a is modified, the unit cell is similarly modified, thus ensuring that the cross sections for the material are appropriately processed. Cell-weighted materials may now be included in the searches, updating the geometry, material, and cross sections as the search progresses.

Several new geometry and array types have been added to KENO-VI. New geometry types include X-cylinder, Y-cylinder, Z-cylinder, pentagon, X-plane, Y-plane, and Z-plane. Three additional array types are available: dodecahedral, which is a three-dimensional (3-D) stack of dodecahedrons; standard hexagonal, which differs from the current hexagonal array type as shown in Figures 1 and 2; and rotated hexagonal, which is a standard hexagonal array rotated 90 degrees (Figure 3).

3. New Modules in SCALE 5

The following sections describe the modules that are being released in SCALE 5.

3.1 CENTRM: Continuous Energy Flux Spectra for Multigroup Cross Sections

The resolved resonance processor modules CENTRM[3] (**C**ontinuous **En**ergy **Tr**ansport **M**odule) and PMC (**P**ointwise **M**ultigroup **C**onverter) provide a significant new capability in SCALE 5. CENTRM is a one-dimensional (1-D) discrete ordinates code that uses a pointwise continuous energy cross-section library to produce a set of pointwise continuous energy fluxes at discrete spatial intervals for each unit cell. Using these fluxes, PMC collapses the pointwise continuous energy cross sections into multigroup cross sections for each nuclide in each material in the unit cell. CENTRM can be used to explicitly model fuel or absorber materials in subdivided regions, such as concentric rings in a fuel pin, to more precisely model the spatial effect on the flux and cross sections. Other modules in SCALE 5, such as KENO, can then use these multigroup cross sections.
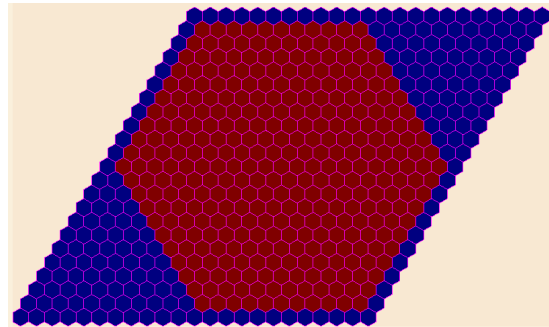

Fig. 1 Hexagonal array (SCALE 4.4a and SCALE 5).
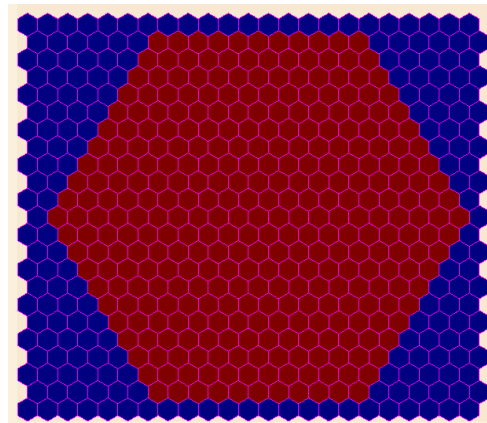
Fig. 2 Standard hexagonal array (SCALE 5).
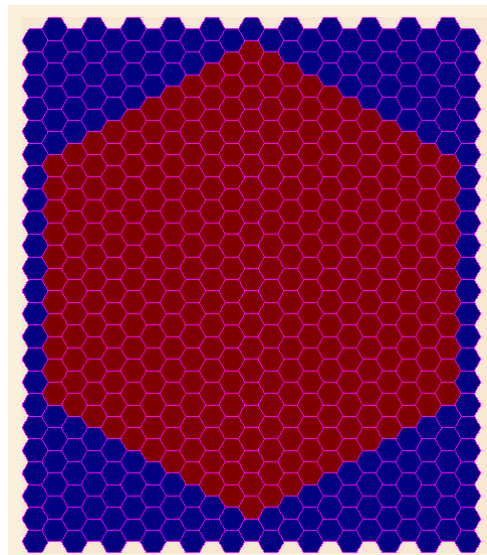
Fig. 3 Rotated hexagonal array (SCALE 5).

Discrete-level inelastic cross-section data can also be processed by CENTRM/PMC. Down-scattering from inelastic continuum data and thermal up-scattering into the pointwise range are optionally available by a multigroup treatment. CENTRM/PMC avoids many of the inherent assumptions in NITAWL by calculating a problem-dependent flux profile, thus making it a far more rigorous cross-section treatment. Effects from overlapping resonances, fissile material

in the fuel and surrounding moderator, anisotropic scattering, and inelastic level scattering are explicitly handled in CENTRM/PMC.

A separate set of CENTRM and PMC input files is required for each unit cell. For a SCALE sequence utilizing CENTRM/PMC, the control module produces the input files for CENTRM and PMC based on the unit cell data specified in the problem. If a lattice unit cell is specified, the code converts the cell description to an equivalent Wigner-Seitz cell for processing. When the CENTRM/PMC option is specified, the WORKER utility module is initially run to produce a working format cross-section library. Then CENTRM and PMC are executed for each unit cell specified plus an additional time to process all the nuclides contained in materials not specified in a unit cell. When all nuclides have been processed, WORKER is called again to convert the final master format library to a working format library.

3.2 TSUNAMI: Sensitivity and Uncertainty for Criticality Safety Analyses

ORNL has invested a significant effort in the development of sensitivity and uncertainty (S/U) analysis capabilities for criticality safety. Both 1-D and 3-D sequences plus several auxiliary codes have been developed into a new suite of S/U analysis codes called TSUNAMI (**T**ools for **S**ensitivity and **UN**certainty **A**nalysis **M**ethodology **I**mplementation).[4,5]

TSUNAMI contains a number of codes that were developed primarily to assess the area of applicability of benchmark experiments for use in criticality code validations. However, the S/U data produced by these codes can be used in a wide range of studies. Sensitivity coefficients produced by the TSUNAMI sensitivity analysis sequences predict the relative changes in a system's calculated k_{eff} value due to changes in the neutron cross-section data. TSUNAMI produces sensitivity data on a groupwise basis for each region defined in the system model. The TSUNAMI-1D control module generates sensitivity coefficients using XSDRNPM. The TSUNAMI-3D control module is based on KENO V.a.

Both TSUNAMI-1D and TSUNAMI-3D fold the sensitivity data with cross-section covariance data to calculate the uncertainty in the calculated k_{eff} value due to tabulated uncertainties in the cross-section data. Multigroup cross-section covariance data libraries for available nuclides and reactions will be included in SCALE 5.

The applicability of benchmark experiments to the criticality code validation of a given application can be assessed using S/U-based integral parameters.[4,6] The TSUNAMI-IP (Integral Parameters) code utilizes sensitivity data and cross-section covariance data to produce a number of relational integral parameters that can be used to assess system similarity. Some example of uses of the TSUNAMI techniques are given in a companion paper.[7]

3.3 SMORES: Material Optimization for Criticality Safety Analysis

A new SCALE control module named SMORES[8] (**S**CALE **M**aterial **O**ptimization and **RE**placement **S**equence) has been developed as part of the Applicable Ranges of Bounding Curves and Data (AROBCAD) Task undertaken by the U.S. Department of Energy Nuclear Criticality Safety Program. The purpose of SMORES is to perform automated 1-D optimization for criticality safety analysis.

The SMORES sequence consists of three major steps that are repeated as needed: (1) preparation of the cross sections and mixing table used for the transport and optimization calculations; (2) 1-D neutron transport calculation of the angular forward and adjoint fluxes; and (3) calculation of effectiveness functions and optimization of the system with respect to a parameter, either the calculated k_{eff} value of a system or the minimum amount of fissile material in a system that will yield a desired k_{eff} value.

The cross-section processing is performed using either BONAMI/NITAWL-III modules or BONAMI/CENTRM/PMC. The processed cross sections are then used to create a problem-dependent self-shielded macroscopic cross-section library that corresponds to the most recent configuration in the optimization process.

The forward and adjoint neutron transport calculations of the system are performed using the XSDRNPM module. This module performs the 1-D criticality calculation that provides the neutron fluxes that are used to determine the effectiveness functions, as well as the k_{eff} of the current system.

Finally, SMORES calls the SWIF functional module, which has been developed at the University of California, Berkeley. SWIF optimizes a specified parameter (k_{eff} or minimum fissile mass) by calculating the effectiveness functions (equal volume replacement reactive worth) using the forward and adjoint fluxes calculated by XSDRNPM and problem-dependent cross sections. Since the optimization process is iterative, the above steps are repeated until convergence is achieved or the maximum number of iterations is reached. If the maximum number of iterations is reached before convergence, a restart option can be used to optionally change the convergence criteria for continued optimization with a new maximum number of iterations. Along with a standard output file, several plot-oriented output files are created to allow rapid processing for visualization using Javapeno (**Java** **P**lots **E**specially **N**ice **O**utput), which is included with SCALE and described in the next section, or other standard plotting packages. Hence, the system k_{eff}, material concentrations, and fissile mass as a function of iteration number can easily be plotted. Figure 4 shows a plot of fissile mass vs iteration for minimum critical mass search.
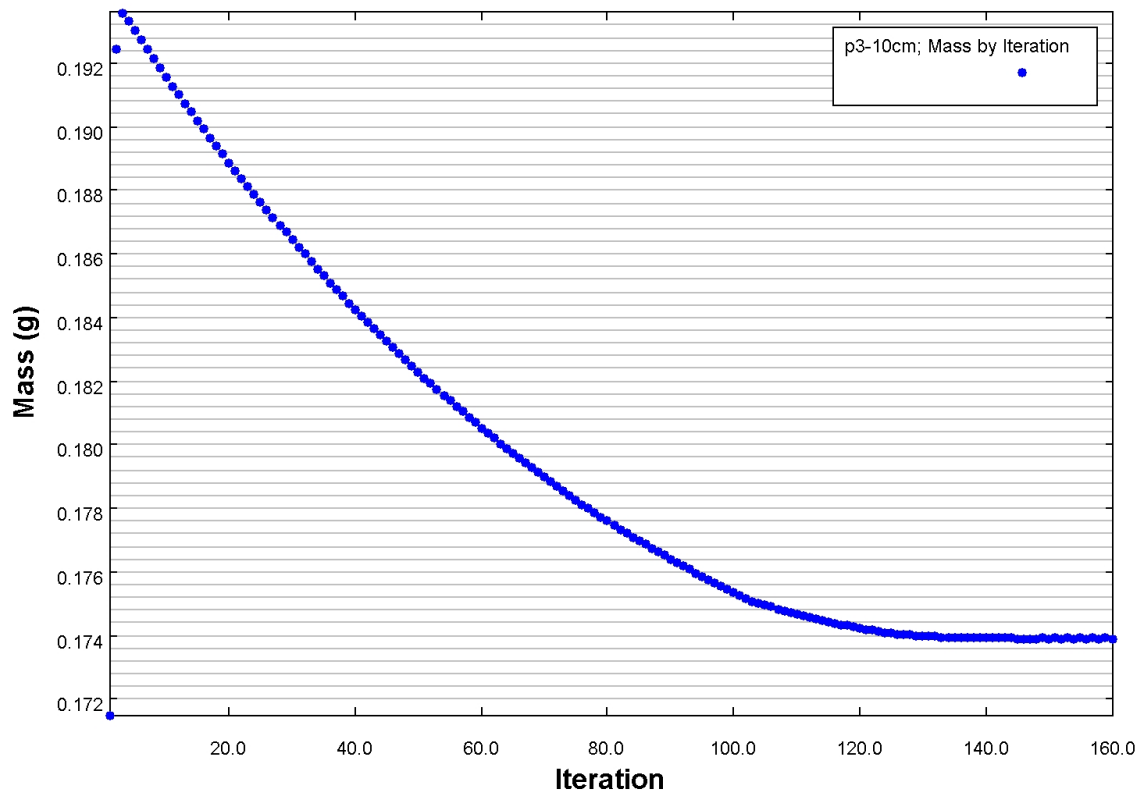
Fig. 4 SMORES minimum critical mass search.

3.4 Javapeno: Interactive Plotting of Calculated Results

Javapeno is a Java program originally designed to plot data from the TSUNAMI sensitivity sequences. It has been expanded to plot the SMORES material optimization sequence results and the groupwise reaction-rate and flux data calculated by KENO V.a/KMART and KENO-VI/KMART6.

Javapeno plots sensitivity, reaction-rate, or flux data as a function of energy group normalized by the unit lethargy for each group, thus eliminating the relative group width from the analysis.

Figure 5 contains a Javapeno plot of the Pu-239 fission sensitivity profiles for two mixed oxide (MOX) polystyrene compact critical experiments.[9] The red curve called nse55t4-01 is the first experiment in Table 4 of that reference, while the blue curve called nse55t5-01 is the first experiment in Table 5 of that reference. The characteristics of these experiments are given in Table 1. The plot shows that the first experiment is much more sensitive to the Pu-239 fission cross section in the thermal range, while the second experiment is much more sensitive in the resonance and fast ranges.

Table 1. MOX polystyrene compact critical experiments

Experiment	nse55t4-01	nse55t5-01
H/(U+Pu)	30.6	2.8
Pu/(U+Pu)	0.146	0.303
wt % Pu-240	7.97	11.5
EALF*	0.143	39.7

*Energy of average lethargy causing fission.

Javapeno plots can be printed directly from the software package or can be exported to a variety of graphics formats to use in reports or presentations. Because of the cross-platform capabilities of Java, Javapeno can execute on any computer for which the Java Runtime Environment is available.
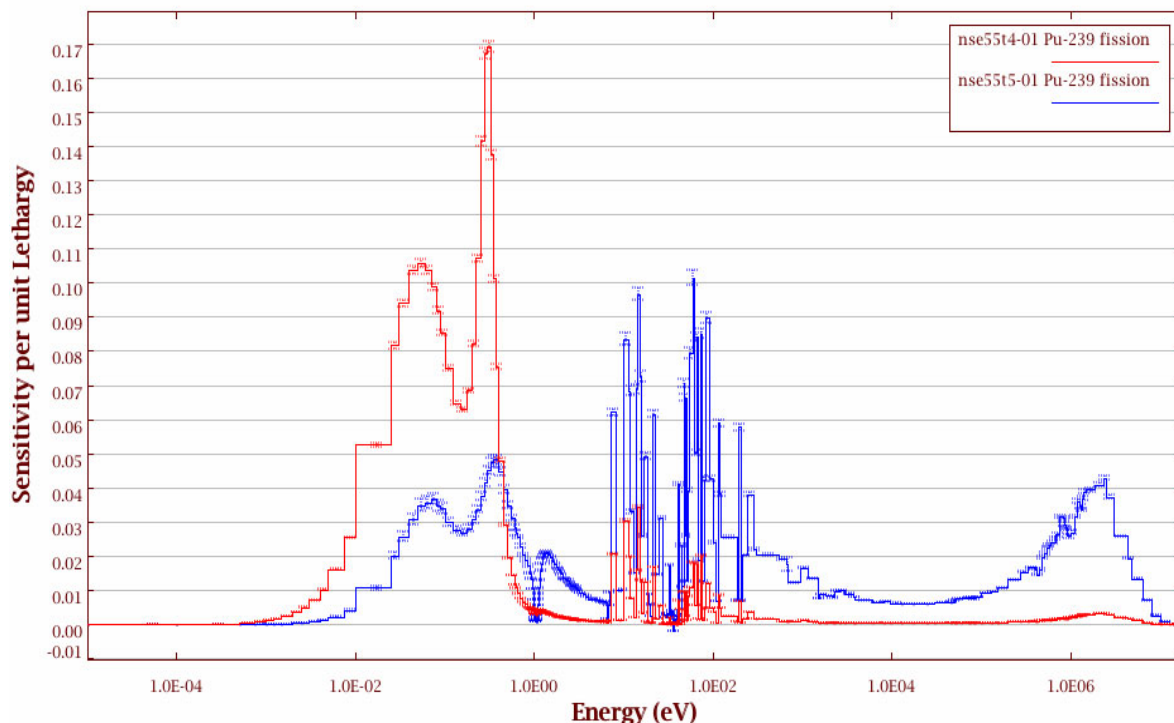
Fig. 5 Javapeno plot of Pu-239 fission sensitivity profiles from MOX polystyrene compact critical experiments.

3.5 STARBUCS: Burnup-Credit Analysis Sequence

STARBUCS[10] (**St**andardized **A**nalysis of **R**eactivity for **Bu**rnup **C**redit using **SC**ALE) is a new sequence to perform criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the criticality analysis of spent fuel configurations by coupling the depletion and criticality aspects of the analysis, thereby eliminating the need to manually process the spent fuel nuclide compositions into a format compatible with criticality safety codes. STARBUCS automatically prepares the input for all codes in the analysis sequence, executes the codes through the SCALE driver, and performs all module interface and data management functions for the user.

STARBUCS performs a depletion analysis calculation for each spatially varying burnup region (if an axial burnup profile is specified) of a spent fuel assembly using the ORIGEN-ARP methodology of SCALE. The ORIGEN-ARP methodology serves as a faster alternative to the SAS2H depletion analysis sequence in SCALE, while maintaining calculational accuracy. The spent fuel compositions are then used to generate resonance self-shielded cross sections for each burnup-dependent fuel region using the SCALE **C**riticality **S**afety **A**nalysis **S**equence (CSAS). Finally, a KENO V.a or KENO-VI criticality calculation is performed using the spatially varying cross sections to determine the neutron multiplication factor for the system.

The STARBUCS control module is designed to facilitate burnup-credit criticality analysis by automating and linking the depletion analysis and criticality calculations. The input format has been designed around the existing depletion analysis and criticality safety sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel calculation is needed to perform a burnup-credit calculation.

STARBUCS has been designed specifically to allow analysts and reviewers to assess the major burnup-credit phenomena identified in the U.S. Nuclear Regulatory Commission Interim Staff Guidance 8 (ISG8).[11] Specifically, STARBUCS allows the user the following capabilities:

1. An arbitrary axial and/or horizontal assembly burnup gradient can be input. The spatial burnup distribution may be controlled entirely by the user. Optionally, built-in "bounding" axial profiles may be selected by the user. A maximum of 100 axial and 10 horizontal zones may be defined.

2. Any or all of the spent fuel actinide or fission product isotopes may be included in the criticality calculation. The user may select from any of the more than 1000 nuclides in the ORIGEN-S libraries, provided cross sections are available for the KENO calculation. This allows the fission product margin to be readily evaluated.

Optionally, the user may request all nuclides to be included to obtain "best-estimate" results.

3. The burnup calculations can specify any desired operating history. The user may specify the assembly-average specific fission power, cycle lengths, cycle downtime, and post-irradiation cooling time. This allows the user to readily evaluate power history and cooling time effects.

4. Isotopic correction factors may be input to adjust the calculated isotopic inventories to account for known bias and/or uncertainties associated with the depletion calculations.

5. Virtually any arrangement of spent fuel may be simulated. STARBUCS is not restricted to spent fuel transport and storage cask analysis. Any KENO geometry model is permissible. For example, spent fuel arrays in a storage pool could be easily simulated.

3.6 TRITON/NEWT: Flexible Mesh 2-D Discrete Ordinates

SCALE 5 introduces two-dimensional (2-D) analytical capability via the NEWT (**NEW T**ransport algorithm) flexible mesh discrete ordinates code. Unlike traditional S_n codes, NEWT is not limited to Cartesian or cylindrical coordinate systems. NEWT's arbitrary geometry, or flexible mesh, allows users to combine orthogonal, radial, and other more unusual geometry shapes in the same model.

NEWT is unique in the domain of discrete ordinates methods because it is based on a nonorthogonal, flexible mesh scheme that allows accurate representation of complex geometric configurations that are normally impossible to model with discrete ordinates methods without significant approximations.[12] Using a discrete ordinates approximation to the transport equation on an arbitrary grid, NEWT provides a robust and rigorous deterministic solution for nonorthogonal configurations. Lower-order deterministic methods typically applied in lattice analyses (e.g., integral transport and collision probability methods) do not provide the angular resolution necessary to treat strongly anisotropic fluxes, such as those in the vicinity of strong absorbers or in high-leakage cores. This limitation may be exacerbated in MOX fuels due to the increased sensitivity of such fuels to the thermal spectrum. NEWT has already been used to demonstrate the effect of minor assumptions on the thermal spectra of MOX fuels.[13]

NEWT offers several calculational options. It may be used to calculate the eigenvalue of a system, to perform a fixed source calculation, or to calculate the critical (X-Y) buckling of a lattice. It allows the specification of an axial buckling or calculates an axial buckling from a specified height to account for axial leakage effects. NEWT can collapse cross sections to an appropriately weighted group structure subset, in the form of an AMPX working-format library.

NEWT's automated grid-generation scheme, based on the placement of simple bodies within a problem domain, allows rapid development of a model without the need to manually input a complex and irregular grid structure. Figures 6 and 7 show two computational grids generated by NEWT for a hypothetical fuel assembly. The geometry input specifications are identical, but a more refined grid is specified for the second model. Note that these models contain no curved surfaces but instead consist of arbitrary polygons computed by NEWT in which volumes are conserved.
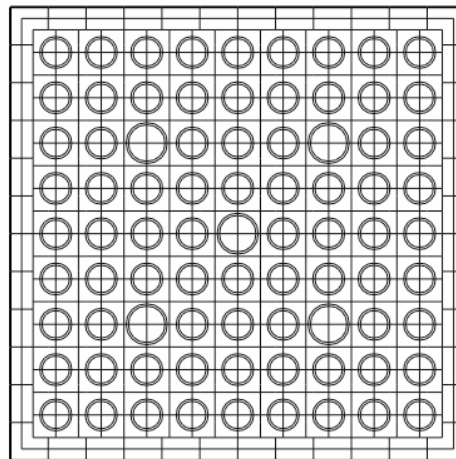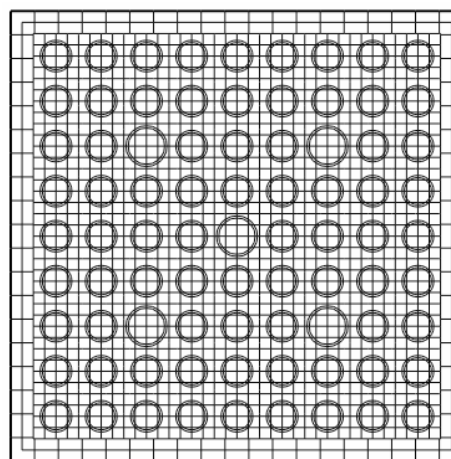

Fig. 6 NEWT coarse grid for fuel assembly.

Fig. 7 NEWT refined grid for fuel assembly.

The TRITON control module (originally developed as a prototype named SAS2D) performs the task of coordination of data transfer between various physics codes, and in invoking those codes in the proper sequence for a desired calculational type.[14] TRITON brings to NEWT the automated and simplified approach for setting up and performing complex sets of calculations, a hallmark of the SCALE system. TRITON provides multiple sequence options, depending on the nature of the problem to be analyzed,

including a single NEWT transport calculation (with problem-specific multigroup cross-section generation) and a 2-D depletion calculation that iterates between NEWT-based transport calculations and ORIGEN-S depletion calculations. The rigor of the NEWT solution in estimating angular flux distributions combined with the world-recognized accuracy of ORIGEN-S depletion gives TRITON the capability to perform rigorous burnup-dependent physics data with few implicit approximations. Such rigor may be necessary to capture the unique attributes of MOX fuel behavior as well as that of advanced, highly heterogeneous fuel assembly designs being deployed in current-generation reactors.

4. Conclusions

SCALE 5 contains many new capabilities for criticality safety analysis, including continuous energy flux spectra for processing multigroup problem-dependent cross sections, ENDF/B-VI resonance processing for multigroup cross sections, 1-D and 3-D S/U analyses for criticality safety evaluations, 2-D flexible mesh discrete ordinates code; automated burnup-credit analysis sequence, and 1-D material distribution optimization for criticality safety. These features will further enhance SCALE's ability to provide a powerful but easy-to-use set of criticality safety analysis tools.

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