



# SCALE Newsletter

Number 34

July 2006

## SCALE 5.1 in Final Testing

The SCALE 5.1 package is currently being tested at the Oak Ridge National Laboratory (ORNL) in preparation for its public release. The release is

anticipated to occur by September 30. Some of the new capabilities of SCALE 5.1 are highlighted in this newsletter. For

more information on improvements to SCALE that will be included in version 5.1, please refer to the January and July 2005 issues.

## New ORIGEN-ARP Libraries in SCALE 5.1

The LWR libraries previously released with SCALE 5.0 were created using the 1-D depletion sequence SAS2. New cross-section libraries have been generated with the 2-D TRITON/NEWT depletion sequence for seven PWR, nine BWR, and five VVER assembly configurations, as listed in Table I. The range of the parameters was extended, as compared with the previous release, to include burnups up to 72 GWd/MTU and fuel enrichments up to 6 wt %  $^{235}\text{U}$ . Unless otherwise noted in Table I, the new libraries were generated for six fuel enrichment values: 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 wt %  $^{235}\text{U}$ . In the case of the BWR assembly designs, five values of coolant density were considered: 0.1, 0.3, 0.5, 0.7, and 0.9 g/cm<sup>3</sup>, whereas for the PWR and VVER a core-average value was used for the moderator density. Three of the four VVER-440 configurations considered are characterized by a radial enrichment profile, and two of these contain burnable absorber rods.

Table I. New LWR libraries for ORIGEN-ARP

Reactor type	Assembly design description
PWR	Westinghouse CE 14 x 14 Westinghouse CE 16 x 16 Westinghouse 14 x 14 Siemens 14 x 14 Westinghouse 15 x 15 Westinghouse 17 x 17 Westinghouse 17 x 17 OFA (Optimized Fuel Assembly).
BWR	GE 7 x 7 GE 8 x 8 ABB 8 x 8 GE 9 x 9 GE 10 x 10 ATRIUM-9 (9 x 9) ATRIUM-10 (10 x 10) SVEA-64 (8 x 8) SVEA-100 (10 x 10)
VVER	VVER-440 flat enrichment 1.6%, 2.4%, 3.6% VVER-440 profiled enrichment, average 3.82% VVER-440 profiled enrichment, average 4.25% VVER-440 profiled enrichment, average 4.38% VVER-1000

### Special points of interest:

- SCALE 5.1 release scheduled for September 30, 2006
- SCALE workshops in Oct./Nov. at ORNL; \$300 discount until September 22

### Inside This Issue:

- New Covariance Libraries for TSUNAMI 2
- KENO-VI Array and Hole Enhancements 3
- GeeWiz/KENO3D Calculate KENO-VI Volumes 4
- Fall 2006 SCALE Training Courses 5

Continued on page 2

## New ORIGEN-ARP Libraries in SCALE 5.1

(continued from page 1)

New ORIGEN-ARP libraries include seven PWR, nine BWR, and five VVER libraries based on 2-D models.

An important aspect of the work was collecting, from various sources, assembly data for each of the designs considered. Because there are small variations in the parameters characterizing the assemblies of a specific design, these gathered data were analyzed in order to build a representative analysis model,

typical for a large number of applications involving assemblies of that type. Most of the assembly information was taken from multiple sources, such as the *2004 World Nuclear Industry Handbook* and various technical reports issued by the U.S. Nuclear Regulatory Commission (NRC) or ORNL. Typical values

were used if data were not available. All PWR assemblies were modeled with no absorber rods/devices inserted into the guide or instrument tubes. The level of detail in the models is illustrated in Fig. 1 for two assembly designs, BWR (GE-9 x 9-7), left, and VVER (VVER-1000), right.

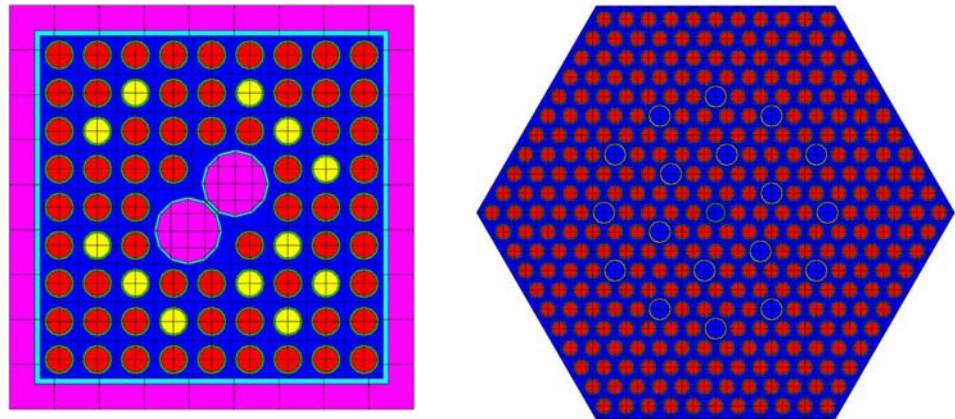


Figure 1

## New Covariance Libraries for TSUNAMI in SCALE 5.1

New covariance libraries contain data for nearly all nuclides in ENDF/B-V and -VI.

For SCALE 5.1, a total of four cross-section covariance libraries are being released; 44GROUPV5COV, 44GROUPV6COV, 44GROUPV5REC, and 44GROUPV6REC. The first two libraries represent a *basic* set with only the covariance data included in the ENDF/B formal release, about 50 nuclides corresponding to ENDF/B-V and ENDF/B-VI, respectively. The last two represent a *recommended* set with covariance information for nearly every nuclide in the cross-section library. The recommended sets contain the ENDF/B-V and ENDF/B-VI data plus a large number of nuclides for which covariance information

is included based on integral uncertainty data. Each of these libraries contains cross-section covariance information in the SCALE 44 neutron-energy-group structure. While conceptually it is possible to process the cross-section covariance information into the SCALE 238 group structure, very little additional information would be available. The capability to use a cross-section covariance group structure that is the same as or a subset of the cross-section library group structure was built into the SCALE sensitivity/uncertainty codes so that these covariance libraries could be used with 238-group calculations.

Each of the four covariance libraries described above processed all of the information that was contained in the cross-section uncertainty files. Because many of the specific reactions that contain uncertainty data are not actually used by the TSUNAMI processing codes, the files were thinned to contain only the reactions utilized by TSUNAMI. These reactions include: total, elastic, inelastic, (n,2n), fission, chi, (n,gamma), (n,p), (n,d), (n,t), (n,He-3), (n,alpha), and nu-bar.

## KENO-VI Array and Hole Enhancements in SCALE 5.1

Recent enhancements to KENO-VI address limitations discussed in the January 2006 issue of the SCALE Newsletter.

As discussed in the January 2006 issue, KENO-VI has certain restrictions that must be observed when using holes and arrays. These restrictions stem from the algorithm used to perform particle tracking through the geometry.

1. Holes may share surfaces with but must not intersect other holes or the boundary of the unit that contains the hole.
2. A hole in a unit contained in an array must not intersect the array boundary.
3. A higher-level array boundary must not cross a nested array boundary.

In SCALE 5.1, KENO-VI has been enhanced to address these limitations. If the first or second restriction is violated, KENO-VI terminates and writes an error message stating why the problem terminated and the unit,

location, and direction of the particle crossing the boundary where the intersection occurs. The third restriction has been removed in SCALE 5.1.

The removal of the restriction on nested array boundaries allows the user to set up complex problems much more simply and avoids the possibility of erroneous  $k_{\text{eff}}$  calculation. For example Figure 2 illustrates where a nested array boundary that overlaps a higher-level array boundary. Because the previous version of the geometry package tracked particles only in the current array level, the particle was required to exit a lower-level array before exiting a higher-level array. In the new version, the particle is tracked in the current array level and all higher-level arrays. This allows the particle to determine the shortest distance to any array crossing and to possibly cross out of multiple arrays simultaneously.

Another example of a problem that can be modeled easily using the new geometry capabilities is a reactor composed of multiple fuel assemblies, each composed of multiple fuel pins, and control blades that move between the assemblies. Each fuel assembly may be set up as an array of fuel pins. The reactor core is then modeled as an array of fuel assemblies with a boundary that consists of the reactor vessel and the control blades. Figure 3 shows an example of this type of configuration. A particle in a fuel assembly crossing into a control blade crosses out of the fuel assembly array and the array of fuel bundles before crossing into a control blade.

These updates highlight our continuing software maintenance efforts to address limitations and potential problems and to make SCALE more accurate and easier to use.

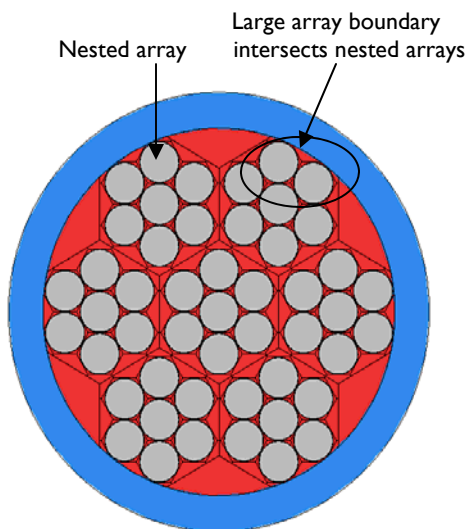


Figure 2

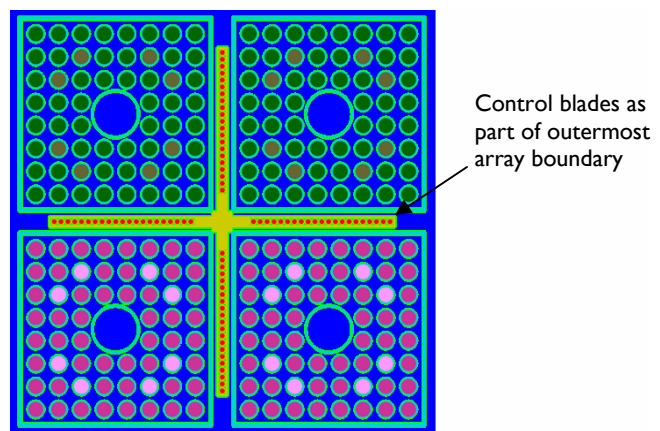
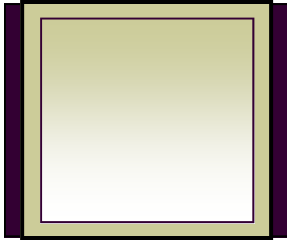


Figure 3

## GeeWiz/KENO3D Calculate KENO-VI Volumes



The SCALE KENO-VI program does not calculate volumes for model bodies by default. The reason is that the calculation of volumes in KENO-VI is more difficult than in KENO V.a due to the generalized geometry in KENO-VI that allows body intersections. Although volumes are not needed for the calculation of  $k_{\text{eff}}$ , they are necessary for the calculation of other parameters such as fluxes and fission densities. They are also required for TRITON6/KENO-VI fuel depletion calculations to correctly normalize the power densities.

The GeeWiz user interface and KENO3D visualization tool have been enhanced to calculate KENO-VI volumes analytically and write those volumes directly to a KENO-VI input file. This new feature is a significant capability that will prove useful for applications that use a KENO-VI (i.e., SCALE Generalized Geometry Package) model and require accurate volumes for model bodies.

KENO3D is a visualization tool that allows users to

interactively view the components of their geometry model as it is constructed. Internally, KENO3D uses constructive solid geometry to build the faceted or wireframe model bodies for display. KENO3D has the capability to calculate volumes of individual bodies. Previously, the volume calculation was used internally by KENO3D when performing Boolean operations (e.g., subtracting bodies and intersecting bodies). With the need for accurate volume calculations for KENO-VI geometry models, the volume calculation was extended to calculate the volumes for each medium in the model and to write the volumes to a file that is formatted for reading by KENO-VI or GeeWiz.

The calculation of volumes in KENO3D has been optimized for models where all units and arrays are bounded by rectangular solids. If a unit or array is bounded by a rectangular solid, then each body can be tested to see if its bounding box intersects that of the rectangular solid. For rectangular geometries, if the bounding boxes do not intersect, then the model bodies do not intersect. If the model bodies do not intersect, then the volume of each object as constructed in its unit of origin is simply added to the accumulated volume for that medium.

The intersection of boxes is significantly faster than the intersection of bodies. For a shipping cask model containing approximately 200,000 bodies, the execution time required to accurately calculate volumes was reduced from 30 minutes to less than 1 second by using the bounding box optimization. With rectangular geometries, when a unit or array bounding box does intersect an object's bounding box, the more-costly calculation using intersections is required for that object. In most practical applications, only a subset of object boundaries intersects unit or array bounds; therefore, execution time would still be reduced by box optimization.

Volumes can be calculated directly with KENO3D; however, as an aid to GeeWiz users, a volume calculation capability was added to the GeeWiz Volume dialog. If the user selects the "Keno3D Volumes" button, KENO3D is called to calculate volumes and create an ASCII volume file formatted for input into SCALE. Subsequently, if the user selects the "Attach Volumes" button, the volume data will be added directly to the media records in every region in the SCALE input file.

## Corrections and Updates to SCALE 5

The [attached file](#) provides a summary of code and data modifications that have been made to the configuration-controlled

version of SCALE at ORNL since January 2006. These modifications will be available later this year in the SCALE 5.1 release.



# SCALE Newsletter

Number 31

January 2005

## Special points of interest:

- SCALE 5.1 scheduled for 2005
- SCALE workshops in March/April at ORNL; \$300 discount until February 28.

## Inside this Issue:

- Improved BONAMIST and NITAWLST codes for TSUNAMI 3
- New 3-D and improved 2-D depletion with TRITON 4
- Important ORIGEN-S updates 5
- SAMS update 5
- Words to the Wise:** 6
  - Changes in SCALE 5 version of ORIGEN-S
  - Infinite homogeneous medium calculation in CENTRM
- Spring 2005 SCALE training courses at ORNL 7

## Advances in SCALE Development

Significant development efforts continue to be made in the SCALE software system since the release of Version 5 in June 2004. This article highlights some of the advances that are being made in SCALE. There will be a special session on this topic at the American Nuclear Society (ANS) meeting in San Diego, June 5-9, 2005.

### Version 5.1

Several improvements that have recently been completed as part of ORNL's ongoing development activities will be included in

Version 5.1 of SCALE, which is scheduled for release in 2005.

### ENDF/B-VI Data

ENDF/B-VI cross-section libraries, both multigroup and continuous energy, have been developed and tested and will appear in SCALE for the first time in Version 5.1. A 238-group library, corresponding to the SCALE 238-group ENDF/B-V energy-group structure, and continuous-energy cross sections for the CENTRM one-dimensional (1-D) discrete-ordinates resonance-processing code will be included.

### HTML Output

An advanced HTML-formatted output interface has been developed for the Monte Carlo code KENO V.a. In addition to easily navigated and color-coded tables of data, interactive plotting capabilities are available. A version of the SCALE 5 data plotting code Javapeno has been developed that executes within the web browser as a Java applet. Javapeno compatible data files are created by KENO V.a. so that the user may view data in colorful, interactive, and customizable plots (Fig. 1).

(See Advances in SCALE page 2)

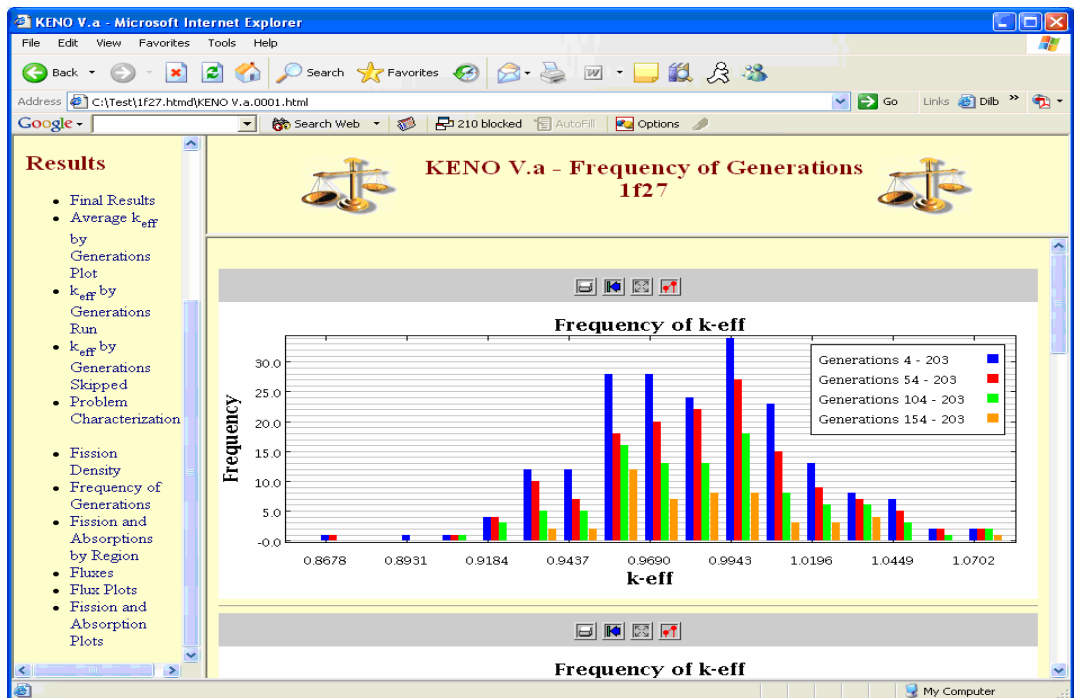


Fig. 1 KENO Frequency of K-eff plot in HTML output.

## Advances in SCALE

Continued from page 1

### CENTRM

- New two-region approximation allows faster self-shielding computations for many problems.

- Unit cell calculations for doubly heterogeneous fuel lumps.

### CENTRM

The introduction of ENDF/B-VI data in SCALE 5.1 will rely heavily on using continuous-energy CENTRM transport calculations instead of NITAWL for resonance self-shielding. (The CPU time required by NITAWL with ENDF/B-VI data is excessively long.) Several important improvements are being made to the CENTRM/PMC codes and the SCALE calculational sequences. The enhancements include improved physics approximations and numerical procedures; more accurate techniques to treat nonuniform arrays and doubly heterogeneous fuel lumps; and a new two-region approximation that allows faster self-shielding computations for many conventional types of problems.

### TRITON

The TRITON fuel depletion module in SCALE 5 has received major upgrades, including the capability to perform three-dimensional (3-D) depletion calculations using the KENO V.a or KENO-VI Monte Carlo codes. In addition, the geometry input for NEWT, the discrete-ordinates code used by TRITON for 2-D depletion, has been replaced with the more versatile SCALE Generalized Geometry Package (SGGP) in KENO-VI. This upgrade improves the portability of input between NEWT and KENO, makes NEWT input for arrays easier, and reduces the input learning requirements for users. (See TRITON article on page 4.)

### TSUNAMI

New and enhanced TSUNAMI (Tools for Sensitivity and

Uncertainty Analysis Methodology Implementation) capabilities for criticality safety in SCALE 5.1 provide a number of advantages over the SCALE 5 implementation. The improved capabilities include

1. analysis of models with more than 50 nuclides with resolved-resonance data;
2. assessment of uncertainty with an improved cross-section covariance data library;
3. processing of ENDF/B-V and -VI data with the new sensitivity version of CENTRM known as CENTRMST; and
4. estimation of biases and uncertainties with TSURFER [Tool for Sensitivity/Uncertainty (S/U) Analysis of Response Functionals using Experimental Results], a generalized linear least-squares computational tool that combines computed and measured benchmark results and provides an estimate for the computational bias and uncertainty.

### Beyond SCALE 5.1

Other important development activities under way will not be completed before the release of SCALE 5.1 but are expected to be available in the subsequent version of SCALE.

### Continuous Energy KENO

Continuous-energy versions of KENO V.a and KENO-VI have been developed and successfully tested with prototype cross-section data. Additional work remains to improve the efficiency of these

codes in both CPU time and memory requirements. Also, the KENO continuous-energy cross-section data are currently limited to only 50 nuclides, each at only one temperature. These data need to be tested thoroughly prior to creating a complete KENO continuous-energy ENDF/B-VI library of all nuclides at multiple temperatures.

### MONACO

A new general-purpose 3-D Monte Carlo radiation shielding code named MONACO is currently under development. Notable improvements have recently been made in the particle tracking efficiency. Testing and validation of MONACO have been performed using benchmark problem comparisons with MCNP. Good agreement has been achieved between the two codes. In addition to comparing the neutron fluxes calculated by MCNP and MONACO, the CPU times were compared. In this series of benchmarks, for the same number of histories in each code, the CPU time used by MONACO was notably less than that for MCNP. Additional work remains to be done to implement a 3-D automated variance-reduction scheme that has been previously demonstrated with MCNP.

### GEMI-NEWTRN

Another development is focused on eliminating approximations used in current resonance treatments by developing continuous-energy multidimensional transport methods for problem-dependent self-shielding calculations. A new code is being developed that utilizes

(Continued on page 3)

### MONACO

A new general-purpose 3-D Monte Carlo radiation shielding code. Benchmark comparisons vs. MCNP show good agreement and faster execution.

## Advances in SCALE

Continued from page 2

the continuous-energy resonance treatment in CENTRM and the two-dimensional (2-D) discrete-ordinates solver NEWT. This new code, GEMI-NEWTRN (Group and Energy-Pointwise Methodology Implemented in NEWT for Resonance Neutronics), performs continuous-energy, multidimensional resonance self-shielding calculations. Preliminary application to an advanced heterogeneous boiling-water-reactor lattice indicates that the problem-specific 2-D resonance self-shielding calculation may have an impact on the prediction of the lattice spectrum.

### STARBUCS

The STARBUCS burnup credit sequence in SCALE 5 is being

enhanced by the development of an automated search sequence that will perform iterative STARBUCS calculations to generate a burnup/ enrichment loading curve for loading spent fuel in casks or storage pools.

### DORT/TORT

DORT and TORT are 2-D and 3-D, respectively, discrete-ordinates radiation transport codes that were developed at ORNL and are used nationally and internationally, primarily for radiation protection and shielding analyses. Despite their recognized capabilities and numerous organizations' reliance on these codes for bulk shielding analyses, DORT and TORT have not been actively developed or improved in many years. As a result, the codes are in need of

modernization and enhancement, particularly in terms of their user-friendliness. Therefore, efforts have been initiated to address these needs. DORT and TORT have been converted from FORTRAN 77 to FORTRAN 90, and additional related programming modernization is under way. Because the capability exists in SCALE 5 to generate problem-dependent cross sections for use by DORT and TORT, the next planned step is to develop a user-friendly SCALE sequence based on TORT.

## Improved BONAMIST and NITAWLST Codes for TSUNAMI

### TSUNAMI

Limit of 50 resonance nuclides removed from NITAWLST in SCALE 5.1.

One obstacle occasionally encountered in TSUNAMI sensitivity/uncertainty analyses is the limit of 50 nuclides with resolved-resonance data in a system model. This limit is imposed by the NITAWLST code, which produces resonance self-shielded cross sections and their sensitivities to input data, a.k.a. "implicit sensitivities." The 50-nuclide limit was partially imposed by limitations in the GRESS software used for automatic differentiation in NITAWLST. An updated version of GRESS has been developed that increases the previous number of allowed independent parameters from 200 to

10,000. Additionally, the updated version of GRESS provides automatic differentiation of a subset of Fortran 90 source code, whereas the implementation of GRESS used with SCALE 5 would process only Fortran 77. An updated NITAWLST code developed with the new version of GRESS has no limit on the number of nuclides in the system model. Additionally, an updated BONAMIST code, used for producing resonance self-shielded cross sections and their sensitivities to input data for the unresolved-resonance region, has been developed with the new version of

GRESS. Although less restrictive than NITAWLST, the SCALE 5 version of BONAMIST limited analyses to a sum of nuclides and mixtures not exceeding 200. The updated BONAMIST increases this limit to a sum of nuclides and mixtures in a single unit cell not exceeding 10,000. The improved versions of BONAMIST and NITAWLST will be available with SCALE 5.1.

## New 3-D and Improved 2-D Depletion with TRITON

**TRITON/KENO**  
3-D Monte Carlo  
depletion option  
available in  
SCALE 5.1.

Increasing complexity in reactor designs is beginning to require robust geometric modeling capabilities to represent neutron transport in complex configurations. Monte Carlo transport methods offer the flexibility needed for such applications. Two new TRITON automated depletion sequences have been developed to perform Monte Carlo-based depletion using KENO V.a and KENO-VI and are planned for release in SCALE 5.1.

The SCALE utility codes KMART and KMART6, originally developed to post-process KENO calculations, have been adapted to provide collapsed cross sections and fluxes required by TRITON for setting up ORIGEN-S depletion calculations. The KENO restart capability is used to provide an improved starting source for each depletion step, thus further improving calculation times. Ongoing work seeks to study and implement methods using variance reduction techniques to improve the efficacy of iterative depletion based on Monte Carlo transport solutions. Error propagation from the results of Monte Carlo simulations is planned as a key part of the system.

Benchmark calculations have been performed using pressurized water reactor fuel assembly data provided in validation reports of the 1-D SAS2 depletion sequence in SCALE. Benchmark models of the spent fuel assemblies have been developed with both TRITON/KENO V.a (TRITON-K5) and TRITON6/KENO-VI (TRITON-K6). The calculated results compare well with the measured radiochemical spent

fuel assay data and previously calculated SAS2 and TRITON/NEWT (TRITON-2D) results. The validation cases are standard benchmarks to ensure that the Monte Carlo codes have been properly incorporated into the TRITON depletion methodology. Further validation is planned using cases that specifically require 3-D representation to obtain accurate results.

NEWT remains a key element of TRITON. NEWT has continued to evolve as a 2-D deterministic transport solver, and has been demonstrated to be valuable in light water reactor fuel assembly depletion analysis and in generating time-dependent lattice physics parameters for nodal code reactor simulator calculations. NEWT's geometry processing capabilities have been significantly enhanced, providing improved stability in grid generation over the initial release. Input for the new geometry package is a 2-D version of the SCALE Generalized Geometry Package (SGGP) that is used by KENO-VI. NEWT input will be easily generated by users familiar with KENO-VI geometry specifications. The former geometry package will be supported in this update to SCALE but will eventually be phased out.

Another significant improvement in NEWT is a coarse-mesh finite-difference (CMFD) accelerator implemented in the iterative solution. Use of this option considerably increases convergence; speedups of a factor of 10 or more have been measured for lattice calculations with large adjacent reflectors. With CMFD and

other optimizations added to NEWT, speedups of a factor of two or more are commonly observed. Multiple enhancements have been made relative to generation of lattice physics parameters. Numerous modifications have been made to help overcome convergence issues for certain classes of problems. Periodic boundary conditions have been added to NEWT, and support has been added for a "white" non-absorbing medium to apply a white boundary condition to non-rectangular problem boundaries.

A paper on the TRITON-K5 and TRITON-K6 sequences will be presented at the Monte Carlo 2005 Topical Meeting in Chattanooga, Tennessee, on April 17–21, 2005. A paper on lattice physics calculations coupling TRITON and the advanced reactor core simulator code PARCS for MOX core-follow calculations will be presented at the ANS Annual Meeting in San Diego, California, June 5–9, 2005.

**NEWT**  
- More versatile  
SGGP geometry  
package.  
- Computational ef-  
ficiency substan-  
tially improved.