Oak Ridge National Laboratory

SCALE Newsletter

Number 35 January 2007

Special points of interest:

- SCALE 5.1 available from RSICC
- SCALE workshops in March 2007 at ORNL; $300 discount until February 11th.

Inside This Issue:

SCALE 5.1 Released

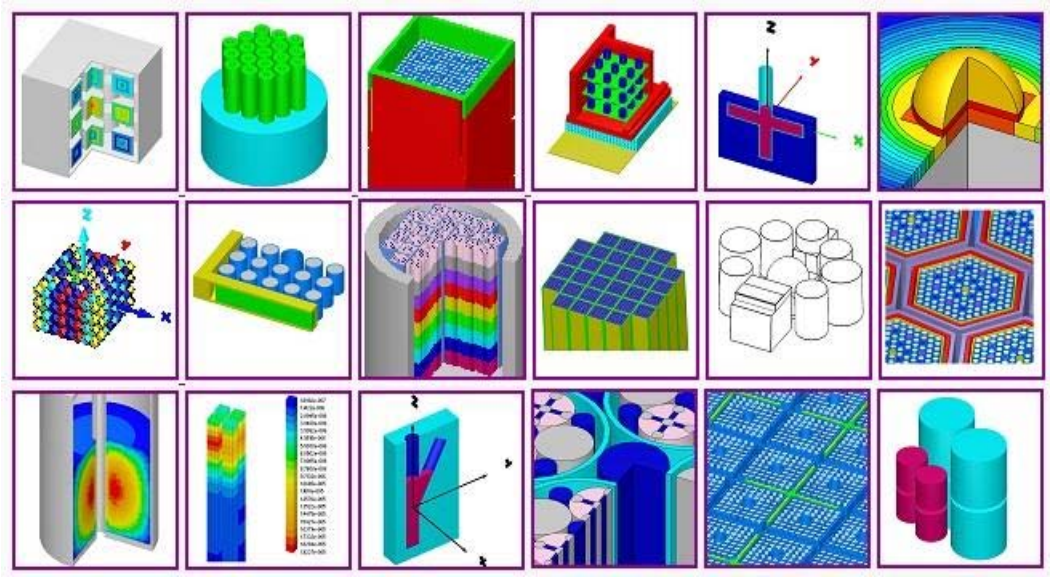
Version 5.1 of SCALE is now available from RSICC. You can order at http://rsicc.ornl.gov/rsiccnew/order.htm or by clicking on the "Order SCALE 5.1" link on the SCALE home page. A summary of new features and capabilities in SCALE 5.1 is provided at http://rsicc.ornl.gov/rsiccnew/SCALE5.1_WhatsNew.pdf, which contains excerpts from previous newsletter issues.

KENO3D 5.1 Free Upgrade

Registered KENO3D 5.0 users may obtain a free upgrade to KENO3D 5.1 by sending an e-mail request to scalecoding@ornl.gov. SCALE 5.1 users who did not purchase KENO3D 5.0 may order KENO3D 5.1 at https://public.ornl.gov/keno3d/index.cfm. The cost of the royalty fee is $100, payable by credit card.

KENO3D Gallery

The KENO3D website contains a gallery of KENO3D images that has been recently updated. We encourage users to visit the new gallery and see some examples of the visualization capabilities of KENO3D. The gallery address is http://www.ornl.gov/sci/scale/keno3d/keno3dgallery.html.



CENTRMST Resource Allocation in TSUNAMI

The TSUNAMI-1D and -3D sequences in SCALE 5.1 use CENTRMST/PMCST to process problem-dependent unit cell data and compute resonance self-shielded cross sections for the resolved resonance region. The "ST" (Sensitivity with TSUNAMI) versions of CENTRM and PMC also compute the sensitivities of the resonance self-shielded cross sections to input data. This so-called "implicit" sensitivity can impact k_{eff} sensitivity results as much as 40%.

The continuous energy solution of CENTRMST can accurately model systems with multiple fuel types, overlapping resonances, and Reich-Moore resonance representations that cannot be fully represented with NITAWLST, the SCALE 5.0 default. However, propagating sensitivities through the CENTRM calculation can come at a significant computational cost.

With the current implementation, CENTRMST uses an algorithm to estimate the number of derivatives that will be generated during execution and allocates an associated amount of memory for use during execution. For many models, the estimated amount of storage space is approximately the same as the actual space required. However, for some models, the amount of estimated space can exceed the amount of space actually required by a factor of 2 or 3. For problems with numerous nuclides in a single unit cell (e.g., spent nuclear fuel), the estimated allocation could be significantly larger than the actual space needed.

CENTRMST prints a message about the amount of memory that it will allocate for derivatives/sensitivities during execution, such as the following:

GRESS will allocate 336000000 locations for derivative storage.

GRESS is the Gradient Enhanced Software System used with the "ST" codes for TSUNAMI. When the code executes successfully, another message is printed near the end of the output detailing how much memory was actually used, for example:

GRESS used 295087416 derivative storage locations of 336000000 available.

When the available memory is insufficient, CENTRMST should print an error message of the following form:

GRESS Error 1: unable to allocate *xxxxx* in *xxxxx* status code is *xx*

where the variable name, subroutine name, and Fortran exit code are given.

However, the Windows executables in SCALE 5.1 built with the Lahey Fortran 95 compiler terminate prematurely and print a cryptic Lahey formatted message in the Run SCALE5.1 DOS window:

jwe0019i-u The program was terminated abnormally with Exception Code EXCEPTION_ACCESS_VIOLATION.

With either message, the workaround is the same. The number of storage locations for derivatives can be modified through the use of the **parm=size=xxx** following the control sequence name in the SCALE input file (e.g., **=ts1d parm=size=xxxx**). The default size for TSUNAMI sequences is 20,000,000. This value is multiplied by problem-dependent factors such as the number of nuclides and the order of scattering. The user may have to perform an iterative search to determine the appropriate size that will allow a large problem to run on a given machine. If the specified size is too small, the calculation will stop when no more space is available, and a message of the following form will be printed:

GRESS Error: Derivative workspace size exceeded. Try reducing the size of the problem or increasing the workspace size with parm=size=###. The current size is *xxxxx*.

If the problem is too large to run on a given machine, other options exist to reduce the computational requirements. Large unit cell models in CENTRMST can produce vast numbers of unknowns. A very fine group flux solution (tens of thousands of energy intervals) must be obtained for each spatial interval. If the size of the unit cell can be reduced, the number of spatial intervals will also be reduced, as will the memory (and execution time) requirements. Also, with the *ISCT* parameter in the CENTRM DATA section of unit cell input, the order of scattering in CENTRMST can be reduced from the default P_3 calculation to P_1 or P_0 with minimal impact to the computed results for most cases.

The SCALE staff plans to improve the sizing algorithm used by CENTRMST in future releases. Please refer to Section M18.5 of the SCALE 5.1 manual for more information on using CENTRMST.

If the problem is too large to run on a given machine, other options exist to reduce the computational requirements.

SCALE 5.1 Updates on the Website

TSUNAMI users should install updates for BONAMIST and GeeWiz.

Installation Files

An update for foreign-language versions of Windows has been posted on the website. Foreign-language Windows users should read page 143 of the SCALE 5 Notebook and install this update.

Tar files for installation of SCALE 5.1 on specific Unix platforms are also available to download. These updates are documented in the SCALE 5 Notebook pages dedicated to SCALE 5.1 installation on these platforms.

TSUNAMI/BONAMIST

An update has been posted to the SCALE website for BONAMIST, which is used by the TSUNAMI sequences to perform resonance self-shielding calculations. This update corrects a minor error in the calculation of background cross sections for reactions other than the total cross section. For most cases the impact is minimal, on the order of 0.01% delta-k. For an extreme case in which most of the reactivity occurs in unresolved resonances (an intermediate spectra MOX fuel with depleted uranium reflector), the impact was a 0.3% delta-k bias. This error is not present in the SCALE 5.0 version of BONAMIST.

TRITON update significantly reduces computational time and memory requirements in PMC.

GeeWiz

A discrepancy has been identified in GeeWiz 5.1. When GeeWiz reads an existing TSUNAMI-1D or -3D input file that contains "PARM=NITAWLST" or "PARM=CENTRMST," it drops the "ST" from the PARM flag and changes it to "PARM=NITAWL" or "PARM=CENTRM," respectively.

An updated version of GeeWiz that corrects this error will be posted to the SCALE website in February. Until the update is available, TSUNAMI users should always specify the PARM= field on the GeeWiz general input screen when reading an existing input file.

TRITON/NEWT/PMC

Updates for TRITON, NEWT, and PMC will be posted to the SCALE website in early February, including enhancements and minor bug fixes. Changes in each code are described below.

TRITON has been updated to reduce the computational time and memory required by PMC during depletion calculations. TRITON automatically adds a large number of additional nuclides in trace quantities to facilitate cross-section updates for depletion. PMC can spend a significant amount of time and require large amounts of memory in preparing weighted multigroup cross sections for such nuclides. However, these low-density nuclides are effectively infinitely dilute and can be treated as such and omitted from PMC processing. By default, TRITON now scans the nuclide concentrations within each mixture and identifies those nuclides that have a concentration of less than a cutoff relative to the largest number density in that mixture. By default, the cutoff has a value of 1e-8, but this value can be overridden by user input. Note that the cutoff is assessed at each time step, such that nuclides that are initially present in trace quantities but build up with depletion are automatically added to PMC calculations once their concentrations exceed the cutoff value.

NEWT has been updated to fix a problem that occurs in printing the input summary within T-NEWT calculations on Linux-based systems. Additionally, NEWT now supports the use of mixture ID 0 (zero) as a void mixture, as is permitted in KENO and XSDRN calculations.

PMC was updated simply to support the update in TRITON described above; the new version of TRITON requires use of the new version of PMC for the calculation to run.

Validation Input Files

Criticality-safety-validation input files for the following validation reports have been updated for compatibility with SCALE 5.1: *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*, NUREG/CR-6361; *CENTRM Validation*, ORNL/TM-2004/66; and *KENO-VI Validation*, ORNL/TM-2004/60. They are also compatible with SCALE 5.0. These can be found on the SCALE Validation web page.

Words to the Wise…

Don't Use V6-238 ENDF/B-VI Library with NITAWL

Updated versions of CSAS and TRITON that prevent use of NITAWL with V6-238 library will be available to download in February.

Users should be aware that the new V6-238 ENDF/B-VI multigroup library in SCALE 5.1 is intended for use only with CENTRM/PMC. It should **not** be used with NITAWL. The Reich-Moore resonance parameters were omitted from the 238-group ENDF/B-VI library because NITAWL required excessive run times to process them. Since the Reich-Moore parameters are not present, NITAWL will run fairly fast with this library. However, it passes infinitely dilute cross sections for nuclides that have Reich-Moore parameters in ENDF/B-VI. If users override the default in SCALE 5.1 and force resonance calculations with NITAWL using ENDF/B-VI cross sections, they can potentially get wrong answers. In previous versions of SCALE, NITAWL was the default module for resonance processing, but there was no ENDF/B-VI-based multigroup library. In SCALE 5.1, CENTRM is the default resolved resonance-processing module to prevent this problem from occurring. Therefore, no problem occurs with the use of existing input files in SCALE 5.1. This scenario could only occur if users change the cross-section library to V6-238 and specify "PARM=NITAWL" to use NITAWL for the resolved resonance range. The SCALE manual clearly states that the CENTRM/PMC modules must be used for the V6-238 ENDF/B-VI multigroup library. Further, GeeWiz does not give users the option to specify NITAWL if the V6-238 library is chosen.

C-12 Not Allowed with CENTRM

When using the SCALE 44- and 238-group ENDF/B-V libraries and NITAWL, both "C" and "C-12" (nuclide IDs 6000 and 6012, respectively) are allowed in the SCALE standard composition input. However, when using CENTRM with the ENDF/B-V libraries or the V6-238 ENDF/B-VI library, only "C" (nuclide 6000) is valid. The CENTRM continuous-energy cross sections for carbon are labeled 6000 for natural carbon because the carbon in ENDF/B is actually natural carbon. However, for historical reasons it was labeled as carbon-12 (6012) in SCALE prior to Version 5.0. The carbon (6012) cross sections in the SCALE ENDF/B-V libraries were copied to natural carbon (6000), and the standard composition library was modified to reference 6000 instead of 6012 for "C" prior to the release of SCALE 5.0.

Dividing the nuclides into multiple CENTRM/PMC runs requires less memory than processing all nuclides in a single CENTRM/PMC case.

Reducing CENTRM Memory Requirements

CENTRM can require a significant amount of computer memory, especially if a large number of nuclides are included in the input (e.g., TRITON depletion or a burnup credit case). If the memory requirements exceed the available physical memory, data may be paged to the hard disk, which will cause the problem to run very slowly. In some cases, the memory requirements may exceed what the computer system can provide and the job will terminate.

Note that separate CENTRM/PMC cases are run for each unit cell (LATTICECELL, MULTIREGION, or INFHOMMEDIUM) specified in a CSAS, TRITON, or TSUNAMI input file. All nuclides not included in a unit cell are processed in a single CENTRM/PMC case using INFHOMMEDIUM.

Dividing the nuclides into multiple CENTRM/PMC runs requires less memory than processing all nuclides in a single CENTRM/PMC case. To work around an insufficient-memory problem, users can use explicit INFHOMMEDIUM unit cell data for some mixtures to reduce the memory requirements.

More Words to the Wise…

Temperature Effects with CENTRM

Some k-eff calculations for LWR fuel at operating temperatures are approximately 0.5–1.0% lower using CENTRM/PMC computed using NITAWL and the ENDF/B-V libraries.

In SCALE 5.1 the default resonance self-shielding method was changed from NITAWL to CENTRM/PMC. Approximately 250 critical, room-temperature benchmarks were used to validate the new methodology, and CENTRM/PMC was generally found to give as good or better agreement with the experimental results as NITAWL. However, there is only limited experience with using CENTRM/PMC for reactor operating conditions and for fuel depletion. Recently it has been observed that some k-eff calculations for light water reactor (LWR) fuel at operating temperatures are approximately 0.5–1.0% lower using the default CENTRM/PMC treatment than values computed when using NITAWL and the ENDF/B-V libraries. LWR pin-cell calculations with XSDRNPM, NEWT, and KENO all show the same trend. ORNL has also observed that TRITON depletion calculations using CENTRM may produce isotopic results that do not agree as well with measurements as NITAWL. In particular, it appears that U-238 absorption, and consequently Pu-239 production, are overpredicted.

This phenomenon is being studied by ORNL to determine the cause and the correction needed. Until an update is made, we recommend that NITAWL and the ENDF/B-V libraries be used for all TRITON LWR fuel-depletion models. As noted elsewhere in this issue, NITAWL should not be used with the 238-group ENDF/B-VI library. To use NITAWL in SCALE 5.1, specify PARM=NITAWL on the first input line, immediately after the sequence name, for example:

=T-DEPL PARM=NITAWL

Note that SAS2H is not affected because it only works with NITAWL.

Tips and Tricks for SCALE 5.1 Users

GeeWiz has a new option, "Stop SCALE (cancel execution)," which can also be activated using the shortcut keys Ctrl+Alt+S.

Stop KENO execution on demand

In SCALE 5.1, an option has been added to allow users to terminate KENO V.a or KENO-VI in an orderly manner after the current generation is completed. The calculated results are tabulated for the number of generations completed (after skipping the first NSK generations) so that a user can terminate a calculation early and still get useful results.

The user can do this manually or via GeeWiz. In GeeWiz 5.1, under the File menu is a new option, "Stop SCALE (cancel execution)," which can also be activated using the shortcut keys Ctrl+Alt+S. This option will terminate SCALE for the case that is currently open in GeeWiz.

The user can manually stop execution by placing a file named "**stop_keno**" in the temporary working directory where the SCALE job is executing. There are no requirements on the content of the **stop_keno** file.

Include batch arguments in SCALE input file

In SCALE 5.0 and 5.1, there are several arguments that can be used with the ***batch5*** command to run SCALE. These arguments have been added to GeeWiz 5.1 on the General input screen (Figure 1). GeeWiz writes the arguments that are checked to a comment line in the input file with the following format:

'batch_args \-arg1\-arg2

For the flags checked in Figure 1, the comment line would look like this:

'batch_args \-m \-r \-u

The ***batch5*** command in SCALE 5.1 searches the input file for the keyword "batch_args" and reads those argument flags.

This feature allows the input file to be run on a different computer or in an overnight batch job and still exercise the same options. It also allows SCALE 5.1 users to manually set these flags in their input files.

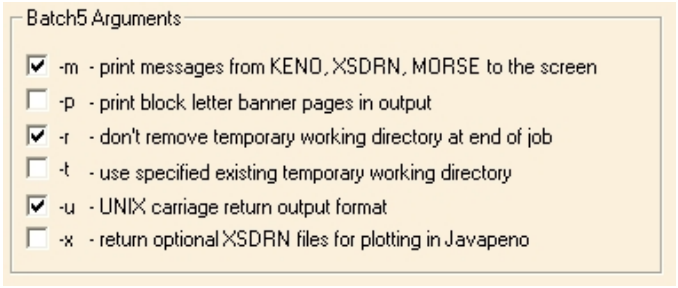


Figure 1. Batch5 arguments on GeeWiz general input screen

New KENO-VI Particle Crossing Algorithm in SCALE 5.1

New KENO-VI particle crossing algorithm is more general and robust.

KENO-VI uses generalized geometry, composed of surfaces that can be represented by quadratic equations, to model the material volumes of a system. There are approximately 20 predefined volumes (e.g., sphere, cylinder, cuboid, cone, wedge, hexprism) that can be combined using rotations and translations. All predefined volumes, except cones, are composed of non-reentrant surfaces. In addition, the generalized quadratic equation can also be used to generate reentrant surfaces. A reentrant surface is defined as a surface on which a particle inside a volume can traverse a straight-line path that crosses the surface and leaves the volume, then later crosses the surface again and reenters the volume. The quadratic equation that defines a conical surface actually defines two infinitely long cones that share an apex (Figure 2). For a finite truncated cone in KENO-VI geometry, the same quadratic equation for the conical surface still applies (with planes added for truncation), so it is possible for a particle to cross this infinite surface more than once in a straight-line path and "reenter" the cone volume (Figure 3).

Continued on page 7

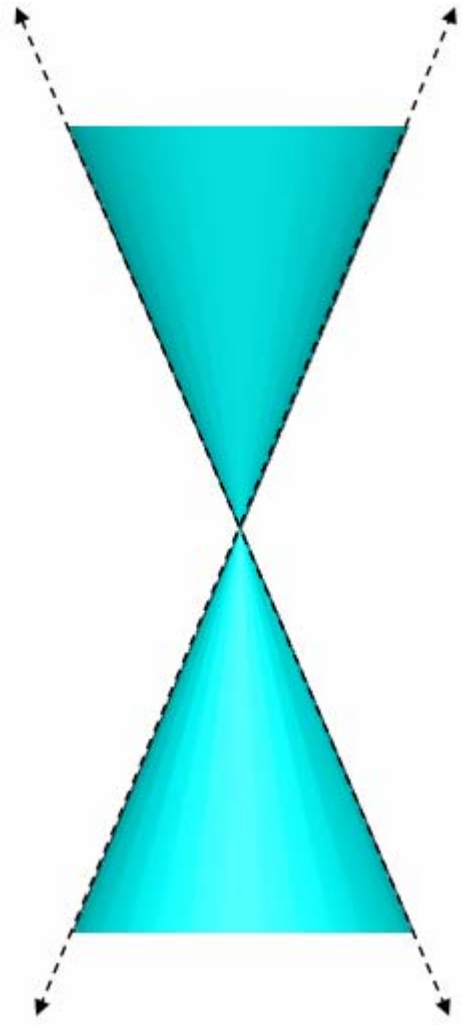


Figure 2. Two infinitely long cones defined by quadratic equation for a conical surface

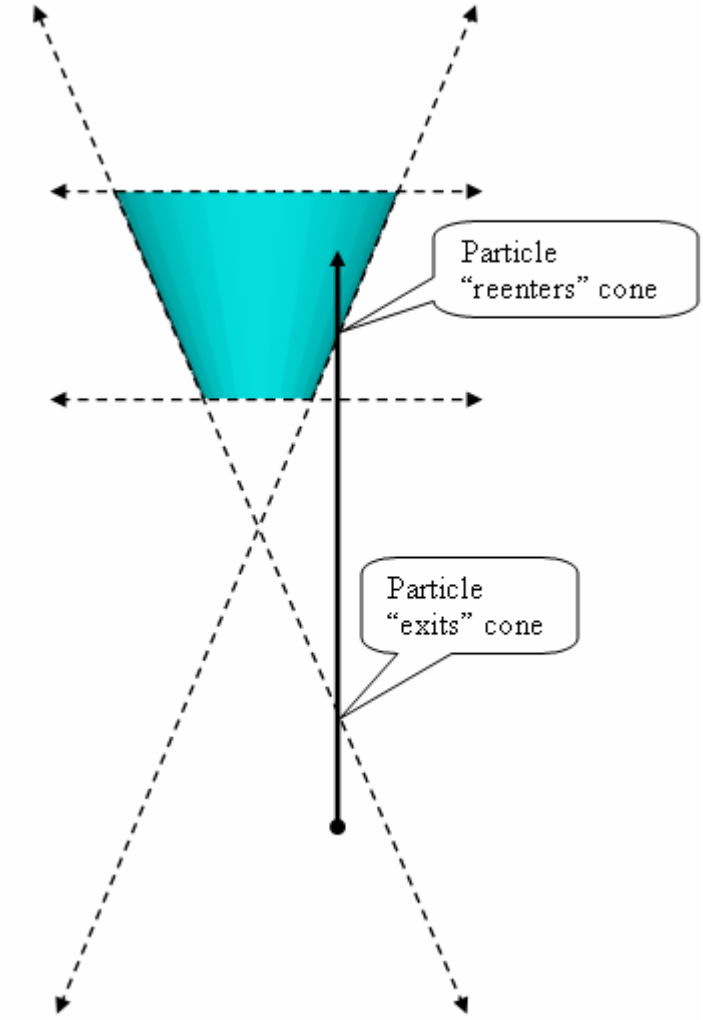


Figure 3. Particle crosses conical surface multiple times and "reenters" the cone volume

New KENO-VI Particle Crossing Algorithm in SCALE 5.1

Continued from page 6

The new crossing algorithm directly uses the quadratic equation to determine the position of the particle.

The potential for problems with reentrant surfaces was discovered recently during a study at ORNL of a high-temperature gas-cooled reactor design that has conical sections in its reactor vessel. To resolve the problem with reentrant surfaces, a new crossing algorithm was developed for SCALE 5.1. When a particle changes direction after a collision in KENO-VI, the crossing distance to every surface in the current unit, plus any array boundaries that contain the unit, must be recalculated. The use of quadratic equations to represent the surfaces means there are two crossing distances per surface. The previous algorithm determined the position of the particle relative to the surface (inside, outside, or on) by examining the crossing distances to the surface. This logic worked well for non-reentrant surfaces but could fail for reentrant surfaces. If it did fail, KENO-VI would enter an infinite loop or terminate with a multiply defined or an undefined region.

The new crossing algorithm directly uses the quadratic equation to determine the position of the particle. The crossing distance is determined by solving the equation for $x+ur$, $y+vr$, and $z+wr$, where x, y, and z define the particle location; u, v, and w are the direction cosines; and r is the crossing distance. It is then a simple matter of solving for r, which has two roots. If one of the two roots of r is zero, the particle is on the surface. If the particle is not on the surface, the position of the particle relative to the surface (inside or out) is determined by the solution of the quadratic equation using the current particle position.

This new crossing algorithm is extremely general and robust. It works for any quadratic equation over a very wide range of particle positions. However, the uncertainty in the crossing distance increases with the size of the system. Models containing units spanning several meters work well. For extremely large units spanning hundreds of kilometers, round-off errors could impact results due to the number of significant figures available for calculating crossing distances.

Wanted: User Feedback on GUI Development

Please post your ideas for SCALE GUI improvements on page 146 of the SCALE Notebook.

ORNL has invested a significant effort into the development of graphical user interfaces (GUIs) for SCALE, such as GeeWiz, KENO3D, OrigenArp, PlotOpus, and Javapeño. We would appreciate feedback from our users on these tools. We have set up a page in the SCALE 5 Notebook entitled "User Forum for Feedback on SCALE GUI Development" for users to post their ideas and exchange thoughts on this topic.

If you have ideas for additional tools/capabilities or how we could make a GUI more user friendly, please post them on page 146 of the SCALE 5 Notebook. If you prefer to submit them privately, you may e-mail them to scalehelp@ornl.gov.

KENO-VI Volume Calculations with KENO3D & GeeWiz

Volumes can be calculated analytically and quickly with GeeWiz and KENO3D using the "KENO3D Volumes" button in GeeWiz.

The SCALE KENO-VI module 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. Volumes are not needed for the calculation of k-eff, but 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.

Note that in previous versions of SCALE, KENO-VI would print fluxes and fission densities based on a volume of 1.0 for each region if volumes were not input or calculated. Because these values were non-physical, the code was modified in SCALE 5.1 to use -1.0 so that users would not mistake these for valid values.

The options for calculation or input of volumes in KENO-VI have been improved for SCALE 5.1 and include two statistical methods: TRACE (ray tracing) or RANDOM (Monte Carlo sampling). In addition, the KENO3D visualization tool has been enhanced to calculate KENO-VI volumes analytically (i.e., exactly) and write those volumes directly to a KENO-VI input file. The volume calculation in KENO3D has been optimized so that it takes only a few seconds in most cases, even for very complex models. 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 will be called to calculate volumes and create an ASCII volume file formatted for input into SCALE. Subsequently, if the user selects the "Attach Volumes" button, GeeWiz will add the volume data directly to the media records in every region in the SCALE input file. This is the recommended method for most cases.

For more details on how to do this, see page 33 in the KENO3D Notebook.

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 July 2006. As indicated in the attachment, most of these modifications were included in the SCALE 5.1 release.

Spring 2007 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
March 5–8, 2007	**TSUNAMI Sensitivity/Uncertainty Tools (Experienced KENO users only)**	$1800
March 12–16, 2007	**ORIGEN-ARP / TRITON Course**	$1800
March 19–23, 2007	**KENO-VI Course**	$1800

*A late fee of $300 will be applied after February 11, 2007.
A discount of $300 for each additional week will be applied for registration in multiple courses.
Foreign nationals must register at least 40 days in advance to obtain security clearance.

For more information and online registration, please visit http://www.ornl.gov/sci/scale/training.htm.

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