Oak Ridge National Laboratory

SCALE Newsletter

Number 30 July 2004

Special points of interest:

- SCALE 5 is now available
- SCALE workshops in October/November at ORNL; $300 discount until September 24

Inside this Issue:

SCALE 5 Is Released by RSICC

Version 5 of the SCALE computer software system developed at Oak Ridge National Laboratory (ORNL), was released in June. This release marks the most significant upgrade to SCALE in more than a decade. Listed below are brief summaries that highlight the capabilities of the new modules and sequences in SCALE 5.

CENTRM

The most significant enhancement to SCALE's cross-section processing capabilities is the new CENTRM (**C**ontinuous **En**ergy **Tr**ansport **M**odule) continuous energy module. CENTRM is a 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, an auxiliary code PMC (**P**roduce **M**ultigroup **C**ross sections) collapses the pointwise continuous energy cross sections into multigroup cross sections for each nuclide in each material in the unit cell. Other modules in SCALE 5, such as KENO, can then use these multigroup cross sections. SCALE 5 also includes pointwise continuous-energy ENDF/B-V cross-section libraries that correspond to the 44-group and 238-group ENDF/B-V libraries. This update permits the coupling of the continuous-energy resonance self-shielding calculation with the multigroup transport solution. CENTRM/PMC provide multigroup cross sections with the accuracy of continuous energy data.

TSUNAMI

Both 1-D and 3-D sequences plus several auxiliary codes have been developed into a new suite of sensitivity/uncertainty (S/U) analysis codes called TSUNAMI (**T**ools for **S**ensitivity and **UN**certainty **A**nalysis **M**ethodology **I**mplementation).

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 neutron cross-section data. TSUNAMI produces sensitivity data on a groupwise basis for each region defined in a system model.

The applicability of benchmark experiments to the criticality code validation of a given application can be assessed using S/U-based integral indices. The TSUNAMI-IP (Indices and Parameters) code utilizes sensitivity data and cross-section covariance data to produce a number of relational integral indices that can be used to assess system similarity.

SMORES

The new control module named SMORES (**S**CALE **M**aterial **O**ptimization and **RE**placement **S**equence) has been developed to perform automated 1-D optimization for criticality safety analysis. SMORES performs optimization of the system with respect to a parameter, either (1) the calculated k_{eff} value of a system or (2) the minimum amount of fissile material in a system that will yield a desired k_{eff} value.

Javapeno

Javapeno (**Java** **P**lots **E**specially **N**ice **O**utput) is a Java program originally designed to plot data from the TSUNAMI sensitivity sequences. It has been expanded to plot SMORES material optimization sequence results and 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. Because of the cross-platform capabilities of Java, Javapeno can execute on any computer where the Java Runtime Environment is available.

NEWT

NEWT (**N**ew **E**SC-based **W**eighting **T**ransport code) is a flexible mesh discrete

(See SCALE 5 page 2)

SCALE 5

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Multiple Unit Cells
SCALE 5 allows multiple unit cells for problem-dependent cross-section processing. Any number of unit cells may be specified, but each mixture number may appear in only one unit cell.

ordinates code. Unlike traditional S_n codes, NEWT's arbitrary geometry, or flexible mesh, allows users to combine orthogonal, radial, and other more unusual geometry shapes in the same model. 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.

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.

TRITON

The TRITON control module 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 the capability to generate few-group cross-section data for use in subsequent nodal diffusion calculations.

TRITON provides multiple sequence options, depending on the nature of the problem to be analyzed, e.g., a single NEWT transport calculation (with problem-specific multigroup cross-section generation) or ORIGEN-S depletion calculations that iterate between NEWT-based transport calculations.

However, in a departure from the traditional province of SCALE applications, TRITON provides the capability to generate few-group cross-section data for use in subsequent nodal diffusion calculations. TRITON supports branch analyses that allow calculation of cross sections and their first derivatives with respect to fuel and moderator temperature, moderator density, soluble boron concentration, and control rod insertion, as a function of burnup. These cross sections are stored in a database format that can be retrieved and processed as appropriate for use by core analysis codes.

STARBUCS

STARBUCS (**St**andardized **A**nalysis of **R**eactivity for **Bu**rnup **C**redit using **S**CALE) 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 performs a depletion analysis calculation for each spatially-varying burnup region of a spent fuel assembly using the ORIGEN-ARP methodology of SCALE. The spent fuel compositions are then used to generate resonance self-shielded cross sections for each burnup-dependent fuel region using the SCALE CSAS control module. 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 input format has been designed around existing depletion and criticality safety analysis sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel criticality safety 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 NRC Interim Staff Guidance 8 (ISG-8).

ORIGEN Updates

The neutron source methods in ORIGEN-S have been significantly enhanced with more rigorous and general methods for the evaluation of spontaneous fission neutrons, neutrons arising from (alpha, n) reactions in an arbitrary matrix, and delayed neutrons arising from short-lived fission products.

Several major nuclear data upgrades have been implemented, including:

(1) replacement of basic neutron cross sections (compiled from 1960's data) with evaluations from ENDF/B-VI, the European Activation File (EAF-99), and FENDL-2;
(2) upgrade and expansion of the fission product yields from ENDF/B-V to ENDF/B-VI, release 2, increasing the number of fission products from 879 to 1110;
(3) expansion of the actinides with explicit fission product yields to 30;
(4) upgrade of the photon emission line-energy data, originally developed for ORIGEN2 in 1985, using ENDF/B-VI and ENSDF photon emission data.

Modeling Fissile Solution Densities with the Pitzer Method in SCALE 5

A longtime feature of the SCALE Material Information Processor Library (MIPLIB) used by the CSAS sequences is the automated calculation of number densities for three fissile solutions: uranyl fluoride, uranyl nitrate, and plutonium nitrate. In assessing the criticality of actinide solutions such as these, highly accurate calculation of the solution density is essential. This is fairly simple for binary solutions where ample data are available; however, it becomes much more difficult if solutions contain many components and are at temperatures other than 25°C. The empirical formulas used in previous versions of SCALE were known to have limitations in this regard.

Another model has been implemented in SCALE 5 for nitrate solutions. The Pitzer method, which has been applied at 25°C to solutions of uranyl nitrate in nitric acid, is used in SCALE 5 to build a model for calculating solution densities involving nitric acid and the nitrate salts of UO_2^{2+}, Th^{4+}, and Pu^{4+}. In general, agreement is within +/-1% relative error. This pattern is also true of most binary systems. The maximum relative error for other ternary systems may be 2-3%, although error for most points is less than 1%. Because this new method works with Th^{4+}, thorium nitrate has been added to the fissile solution densities in SCALE 5. More detailed information can be found in Sect. M7.B of the SCALE 5 Manual.

The model has been validated by recalculation and comparison with data used in the regression process. High accuracy has been demonstrated for nitrate solutions of uranium throughout the range 0–100°C, moderate accuracy for Th solutions in the range 15–60°C, and lower accuracy for Pu solutions in the range 25–60°C. While the model is not proven beyond these ranges, some extrapolation in temperature (15–20% of the listed range) may be acceptable.

The present model is applicable to any solution involving U(VI), Th(IV), or Pu(IV) in nitric acid. All three actinides could be present. It is anticipated that future development will extend these ranges, as new data become available. In addition, the model will include additional actinides and actinide salts involving other anions (e.g., fluoride, sulfate) and additional Pu oxidation states. The ultimate goal is a comprehensive model involving many actinide cations, all relevant anions, and a wide range of temperature.

High accuracy for uranyl nitrate solutions throughout the range 0–100°C

Moderate accuracy for Th solutions in the range 15–60°C

Lower accuracy for Pu solutions in the

How to Order and Install SCALE 5

If you have not already ordered SCALE 5, you can easily do so by going online to RSICC's web page for ordering software, http://rsicc.ornl.gov/rsiccnew/order.htm

Note that RSICC's policy is to issue all software via **single user licenses**. RSICC recently lowered the price of a single license package as part of this policy. The current pricing structure (obtained from the above web page) is listed in the box to the right.

SCALE 5 includes a 30-day trial version of KENO3D. Registered SCALE 5 users can purchase and download the licensed version of KENO3D with the secure online payment of a $100 license fee via credit card at https://public.ornl.gov/keno3d/index.cfm

Installation of SCALE 5 requires online registration to obtain a registration key. The first screen prompts the user for their RSICC pass number and their RSICC password. The second screen requests the computer name (for Windows users) and the RSICC pass number. Unix/Linux users should enter their user ID in the computer name field.

(Note that the SCALE serial number is **not** on the CDs. Your serial number is your RSICC pass number.) The serial number and the registration key are then displayed. Copy and paste these items into the installation form (Windows) or the register script (Unix/Linux).

Be sure to read the file GettingStarted.pdf (Windows) or ReadUnix.pdf (Unix/Linux) for installation instructions. Also check the new SCALE 5 notebook for revisions and additional tips http://www.ornl.gov/sci/scale/scale_notebook.html

RSICC Fees for SCALE 5 (Single User License)

RSICC's DOE/NRC funding offices and their contractors: No charge

Other DOE offices and contractors, government agencies, US educational institutions, Not For Profits: $200

US general public: $300

ALL Non-US installations: $400

GeeWiz: A Complete Graphical User Environment

GeeWiz provides SCALE users with a completely integrated environment for input, output, 3-D visualization, and plotting

One of the exciting new features in SCALE 5 is the **G**raphically **E**nhanced **E**diting **Wiz**ard (GeeWiz). GeeWiz is a Windows graphical user interface that is compatible with

- CSAS/KENO V.a
- CSAS6/KENO-VI
- TSUNAMI 1-D and 3-D.

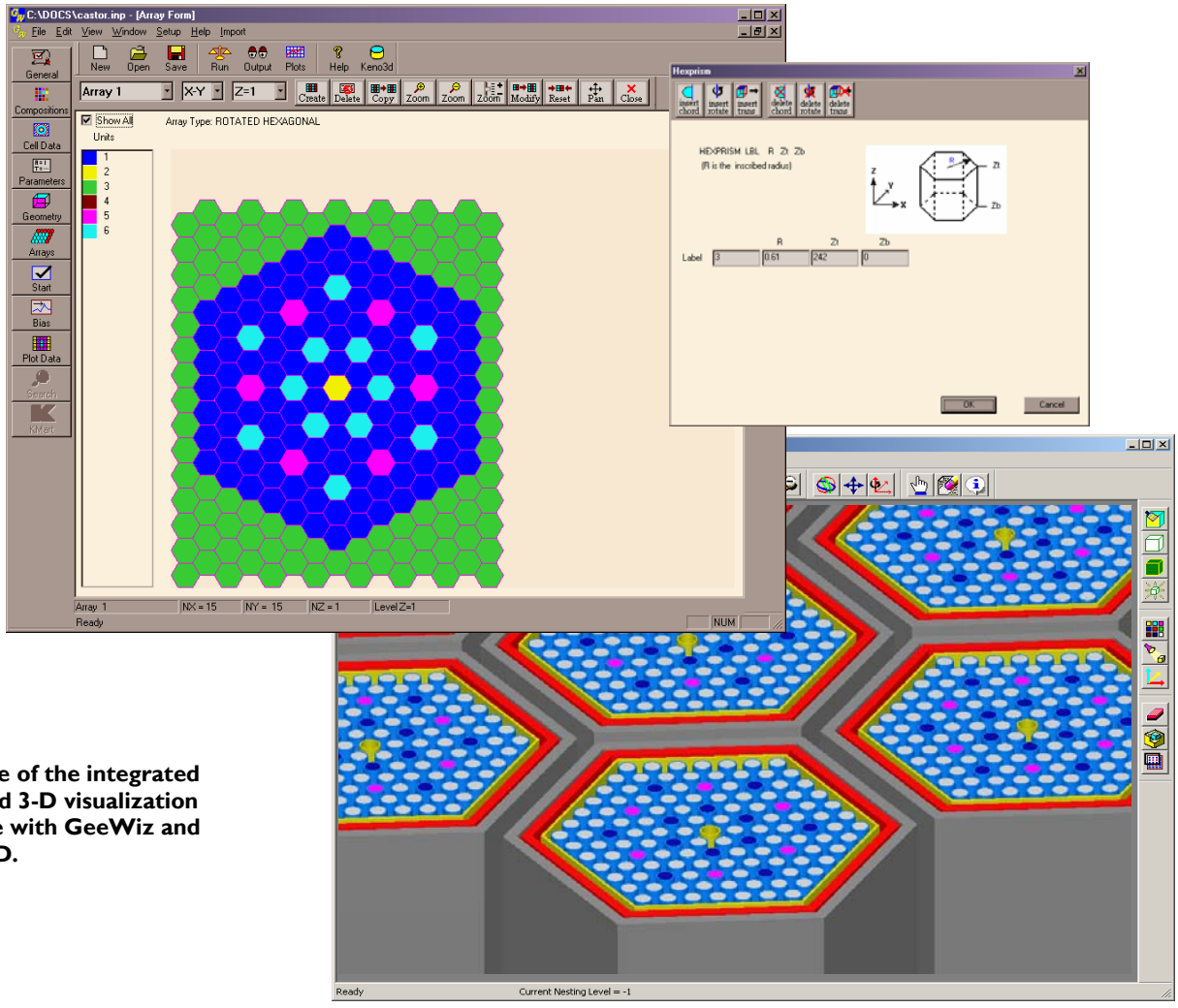
GeeWiz provides input menus and context-sensitive help to guide users through the setup of their input. The user can click a button to call KENO3D and view the components of their geometry model as it is constructed. Once the input is complete, the user can click a button to run SCALE, another button to view the output file, and another button to plot fluxes and reaction rates (calculated by the KENO post processor KMART) and sensitivity data (from the TSUNAMI/SAMS module) with the new Javapeno plotting package in SCALE 5.

GeeWiz is compatible with several important new SCALE 5 features:

- multiple unit cells for cross-section processing,
- new criticality sequences using the CENTRM continuous-energy module, and
- new geometry and array options in KENO-VI.

GeeWiz can read existing SCALE 4 input files and automatically convert them to the new SCALE 5 input format.

Below are some sample screens from a GeeWiz/ KENO3D session.



Example of the integrated input and 3-D visualization available with GeeWiz and KENO3D.

Fall 2004 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
Oct. 25-29, 2004	**SCALE Source Terms and Shielding Course**	$1800
Nov. 1-5, 2004	**KENO V.a Criticality Safety**	$1800
Nov. 8-10, 2004	**TSUNAMI Sensitivity/Uncertainty Tools** (KENO V.a course prerequisite for new users)	$1200
Nov. 11-12, 2004	**STARBUCS Burnup Credit** (KENO V.a course prerequisite for new users)	$1000

*A late fee of $300 will be applied after September 24, 2004.
A discount of $600 per each additional week will be applied for registration to multiple courses.

For more information and online registration, please visit www.ornl.gov/scale/trcourse.html

NSTD The Nuclear Science and Technology Division

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***SCALE Newsletter* is published twice a year by:**
Nuclear Science and Technology Division
Oak Ridge National Laboratory

Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

SCALE Newsletter is sponsored by:
U.S. Nuclear Regulatory Commission, Spent Fuel Project Office
U.S. Department of Energy

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