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Overview of the SCALE TSUNAMI Sensitivity and Uncertainty Analysis Tools

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INTRODUCTION

The Tools for Sensitivity and UNcertainty Analysis Methodology Implementation (TSUNAMI) within the Standardized Computer Analyses for Licensing Evaluation (SCALE) code system provide a number of robust analysis tools for eigenvalue sensitivity and uncertainty analysis in a production-level, publicly available, configuration- controlled package. This paper provides a brief summary of the TSUNAMI capabilities currently available in SCALE 5.1,[1] as well as emerging capabilities for reactor physics and shielding analysis.

SCALE 5.1 CAPABILITIES

SCALE 5.1 contains the most thorough set of tools available for eigenvalue sensitivity analysis, uncertainty quantification, and experiment-to-application similarity assessment for code validation.

Eigenvalue Sensitivity Analysis Capability

The TSUNAMI-3D sequence uses the KENO V.a Monte Carlo neutron transport code to produce the sensitivity of k_{eff} to cross-section data on an energy-dependent, nuclide-reaction-specific basis. In this calculation, the sensitivities of k_{eff} to the problem-dependent multigroup cross-section data are produced with adjoint-based perturbation theory. Problem-dependent resonance self-shielding calculations are performed with automatic differentiation versions of the BONAMI and CENTRM codes that produce not only the appropriate cross-section data but also the sensitivity of the resonance self-shielding corrections to the materials present in the model.[2] When propagated to the k_{eff} sensitivities, the so-called “implicit effect” from the resonance self-shielding calculations can impact results by up to 40%. The automatic differentiation tool, GRESS 90 with code coupling,[3] was used to produce the sensitivity versions of BONAMI and CENTRM.

Uncertainty Quantification

Once the sensitivities of k_{eff} to each energy-dependent, nuclide-reaction-specific cross-section data component have been computed, the TSUNAMI-3D sequence determines an uncertainty in the computed k_{eff} due to tabulated uncertainties for the cross-section data. The cross-section uncertainties are stored in terms of energy-dependent covariance matrices. SCALE 5.1 contains a comprehensive library of uncertainty information for ENDF/B-V and ENDF/B-VI cross-section data. The covariance libraries were developed by processing all available covariance information from the respective library, which is limited to only a few dozen nuclides. For all other nuclides, the integral uncertainty data[4] for thermal and intermediate energies were used to form the required energy-dependent matrices.

TSUNAMI-3D computes the cumulative uncertainty in k_{eff} due to uncertainties in all nuclides and reactions and also tabulates the uncertainty in k_{eff} due to each specific nuclide and reaction. Thus, specific sources of uncertainty can be easily identified.

Code Validation

Numerical codes must be validated against benchmark experiments with characteristics similar to the target application.[5] The TSUNAMI-IP code utilizes sensitivity data from benchmark experiments and target applications along with the cross-section covariance data to numerically quantify the similarity of a benchmark to a target application.

A widely used index for similarity assessment is the correlation of k_{eff} uncertainties, known as c_k. The c_k index quantifies the amount of shared uncertainty in the k_{eff} values of an application and a benchmark due to cross-section uncertainties. A c_k value of 1.0 means that the uncertainties for the application and the benchmark are all generated from the same nuclides and reactions at the same energies, whereas a c_k value of 0.0 means that uncertainties of the two systems are completely unrelated. Parametric extrapolation of the biases of benchmarks relative to c_k provides an accurate prediction of the bias of the target application.

A premise of the TSUNAMI validation concept is that computational biases originate with the cross-section data. If the cross-section uncertainties are correctly tabulated, then computational biases should be bounded by the uncertainties.

Additional capabilities are available in TSUNAMI-IP to assess similarity on a nuclide-reaction-specific basis and to identify specific components of the target application that are not validated by available benchmarks. If inadequacies in the benchmark set are identified, the characteristics of experiments that meet the validation requirements of the target application can be determined from the TSUNAMI data, and optimized new experiments can be designed.[6]

Graphical User Interfaces

A hallmark of the SCALE code system is ease of use. The GeeWiz package provides Window XP users with a convenient means of creating input, executing SCALE sequences, and viewing output for TSUNAMI-3D and many other SCALE computational tools. The output can be viewed as a standard text file or with an interactive HTML interface, which contains integrated data plotting with the Javapeño package.[7] Javapeño is a customized plotting package for SCALE that allows the visualization of sensitivity data, cross-section and cross-section covariance data, as well as fluxes and many other SCALE data types, in an interactive format.

Configuration Control, Documentation, and Training

The most robust software is useless in a licensing environment without accountability. The SCALE package is developed in a configuration-controlled environment and distributed through the Radiation Safety Information Computational Center. SCALE has been used in the Nuclear Regulatory Commission and Department of Energy licensing environment since the 1980s. The input, output, and theory of the SCALE codes are described with over 5000 pages of documentation, and hands-on training with instruction by the code developers is offered in a multiday format twice each year.

EMERGING CAPABILITIES

Several development efforts are currently in progress to further enhance the capabilities of TSUNAMI in improving eigenvalue techniques; utilizing eigenvalue sensitivities to produce reactivity sensitivities; and implementing generalized perturbation theory, shielding perturbation theory, and data-adjustment bias-assessment techniques.

Advanced Monte Carlo Techniques

Currently, the TSUNAMI-3D sequence produces a separate forward and adjoint criticality calculation for each system model. Innovative Monte Carlo techniques are currently under investigation to produce sensitivity data in a single calculation to accelerate calculations and simplify the input requirements for users.

Reactivity Sensitivity

The Tool for Sensitivity Analysis of Reactivity (TSAR) uses a reactivity differencing approach such that the sensitivity data from two eigenvalue calculations can be used to quickly compute the sensitivity of the reactivity difference between two state points to the cross-section data used in their calculations.[8] With the availability of the sensitivity of the reactivity to the cross-section data, uncertainties in the reactivity due to cross-section covariance data can be quantified. Also, the same TSUNAMI-IP techniques used for eigenvalue code validation and experiment design can be applied to reactivity experiments with regard to the target applications for reactor physics code validation.

Generalized Perturbation Theory

To compute the sensitivities of more complex responses, such as burning or breeding ratios to the cross-section data, generalized perturbation theory (GPT) is required. GPT also permits the calculation of reactivity sensitivities directly without eigenvalue sensitivity differencing. The GPT capability was present in the FORSS code system,[9] and development efforts are currently under way to implement this theory in the modern SCALE deterministic transport codes. As with the eigenvalue differencing reactivity sensitivities, once the sensitivities of any response to the cross-section data are available, uncertainties of those responses can be quantified and code validation and experiment design can be conducted.

Shielding Response Perturbation Theory

In a companion paper,[10] new capabilities for shielding sensitivities are described. These observations will not be repeated here.

Data Adjustment for Bias Determination

The Tool for S/U analysis of Response Functionals using Experimental Results (TSURFER) implements a generalized linear least squares approach to consolidate benchmark experiments with computational results by determining adjustments in the cross-section data that maximize consistency between the integral measurements and differential nuclear data. The predicted cross-section adjustments can be propagated to the target application through the appropriate sensitivity data to predict a bias and uncertainty for the calculated target application.

CONCLUSIONS

The production and emerging capabilities of the TSUNAMI tools within SCALE provide robust capabilities for sensitivity and uncertainty analysis, code validation, and experiment design for criticality safety, reactor physics, and shielding applications. The codes are produced in a configuration-controlled environment with convenient graphical user interfaces and data visualization capabilities. Extensive user documentation and hands-on training are also available.

REFERENCES

1. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation,* ORNL/TM-2005/39, Version 5.1, Vols. I–III, November 2006. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732.
2. B. T. REARDEN**,** J. E. HORWEDEL, "Automatic Differentiation to Couple SCALE Modules Using GRESS 90—Part II: Application," *Trans. Am. Nucl. Soc.,* **95**, 702–705 (2006).
3. J. E. HORWEDEL, "Automatic Differentiation to Couple SCALE Modules Using GRESS 90—Part I: Methodology," *Trans. Am. Nucl. Soc*., **95**, 699–701 (2006).
4. S. F. MUGHABGHAB, *Atlas of Neutron Resonances: Resonance Parameters and Thermal Cross Sections Z=1-100***,** Amsterdam, The Netherlands, Elsevier Publishers, 2006.
5. *American National Standard for Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors*, ANSI/ANS-8.1, American Nuclear Society, La Grange Park, Illinois (1998).
6. D. E. MUELLER, G. A. HARMS, "Using the SCALE 5 TSUNAMI-3D Sequence in Critical Experiment Design," *Trans. Am. Nucl. Soc*., **93**, 263–266 (2005).
7. A. M. FLECKENSTEIN, B. T. REARDEN, "Multigroup Cross Section and Cross Section Covariance Data Visualization with Javapeño," *Trans. Am. Nucl. Soc*., **95**, 292–295 (2006).
8. M. L. WILLIAMS**,** J. C. GEHIN, K. T. CLARNO, "Sensitivity Analysis of Reactivity Responses Using One-Dimensional Discrete Ordinates and Three-Dimensional Monte Carlo Methods," *Proceedings of PHYSOR 2006*, Vancouver, Canada, September 10–14, 2006, pp. C135:1–6 (2006).
9. C. R. WEISBIN et al*., Application of FORSS Sensitivity and Uncertainty Methodology to Fast Reactor Benchmark Analysis,* ORNL/TM-5563, Union Carbide Corp., Oak Ridge National Laboratory, Oak Ridge, Tennessee (1976).
10. M. L. WILLIAMS, S. GOLUOGLU, "Sensitivity Analysis for Coupled Neutron-Gamma Calculations," submitted to the American Nuclear Society 2007 Annual Meeting, June 24–28, 2007, Boston, Massachusetts.