TSUNAMI Sensitivity and Uncertainty Analysis Capabilities in SCALE 5.1

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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] which includes 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 identified application.[5] The TSUNAMI-IP code utilizes sensitivity data from benchmark experiments and identified applications along with the cross-section covariance data to numerically quantify the similarity of a benchmark to an identified 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 identified 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 identified 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 identified 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.[7] 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.[8] 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.

CONCLUSIONS

The production-level 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. S. M. BOWMAN, B. T. REARDEN, J. E. HORWEDEL, "Complete User Visualization Interface for KENO," *NCSD 2005 Topical Meeting, Knoxville, TN, September 19–22, 2005*.
8. 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).