User Experiences with ICSBEP Distributed Sensitivity Data Profiles with the SCALE Sensitivity and Uncertainty Methods as of Winter 2019

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INTRODUCTION

A technique using sensitivity uncertainty (S/U) analysis to select critical experiments for use in code validation was developed at Oak Ridge National Laboratory (ORNL) [1] and implemented in the SCALE [2] Tools for Sensitivity Uncertainty Analysis Methodology Implementation (TSUNAMI) code suite. The premise of the TSUNAMI technique is that modern Monte Carlo codes have implemented the transport of neutrons in such an unapproximated way that (1) virtually all of the bias between experiment and calculation is due to errors in the underlying nuclear data and (2) the nuclear data with the highest uncertainties are most likely to be the cause of those biases.

In the TSUNAMI technique, nuclide-, reaction- and energy-dependent k_{eff} sensitivity data are computed for application models and critical experiment models. The sensitivity data are then combined with nuclear data uncertainty information to yield nuclide-, reaction- and energy-dependent k_{eff} uncertainty information for each critical experiment model and safety analysis model. The matrix of covariances of k_{eff} (C_{kk}) due to the nuclear data covariance is given by Eq. (1), where S is the matrix of energy-dependent nuclear data sensitivities for all of the experiments and the applications, and $C_{\propto\propto}$ is the matrix of nuclear data covariances:

$$C_{kk} = SC_{\propto\propto}S^T \tag{1}$$

A correlation coefficient, c_k, indicating the degree to which two systems have similar k_{eff} sensitivity to nuclear data uncertainties, is then calculated for each critical experiment-application pair. A high correlation coefficient value (i.e., c_k approaching 1.0) indicates that the critical experiments and safety analysis models have similar sensitivities to nuclear data with significant uncertainties. The value of c_k for each experiment with each application is calculated using Eq. (2), where σ^2_{appexp} is the covariance of the nuclear data–induced uncertainty between the k_{eff} values of the application. The experiment σ_{exp} is the nuclear data–induced uncertainty in an experiment, and σ_{app} is the nuclear data–induced uncertainty in the application case.

$$c_k = \frac{\sigma^2_{appexp}}{\sigma_{app}\sigma_{exp}} \tag{2}$$

It is noted that σ_{exp} and σ_{app} are the square roots of the diagonal elements of the C_{kk} matrix, and σ^2_{appexp} are the off-diagonal elements of the C_{kk} matrix. In practice, the c_k values are calculated with the TSUNAMI-Indices and Parameters (IP) code, which uses sensitivity profiles calculated with TSUNAMI-3D, a modified version of the KENO Monte Carlo transport code.

From a practical standpoint, performing a similarity assessment between an application and a suite of experiments involves a large amount of time to perform and verify the TSUNAMI-3D transport calculations (several hours to more than a week) to generate the sensitivity data files (SDFs) for the experiments and application. However, the TSUNAMI-IP calculation only requires seconds to several minutes. While generating the SDF for the application model is unavoidable, it is less daunting to generate one SDF compared to the thousands of SDFs that may be needed to produce a suite of experiments similar to the application. In some cases, it may be difficult to know a priori which experiments to model.

Fortunately, some SDFs are distributed with the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook [3]: these SDFs were generated at ORNL for the VALID library [4] and by the Organization for Economic Cooperation and Development through the Nuclear Energy Agency (NEA). The NEA generated a source of readily available SDFs [5], many of which can be used with TSUNAMI-IP. This work documents ORNL's experience using the critical experiment SDFs distributed with the ICSBEP Handbook with SCALE. Items discussed include where to find the SDFs within the file organization of the ICSBEP handbook, the types of calculations for which the provided SDFs are useful, and some useful techniques for manipulating the large number of SDFs using text files.

Location of SDFs

The SDFs distributed with the ICSBEP Handbook are located at `base_location/CD2018/DiceData/` within the file structure, where `base_location` is the location where the user copied all of the data from the ICSBEP Handbook. The directory includes three folders containing sensitivity data: the data generated through the VALID process are located in `/ornl`, the data generated by the NEA are located in the `/sensitivity` subdirectory, and data in the `/ippe` directory were generated at the Institute of Physics and Power Engineering (IPPE).

This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy (DOE). The US government retains and the publisher, by accepting the article for publication, acknowledges that the US government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for US government purposes. DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (http://energy.gov/downloads/doe-public-access-plan).

The ORNL-generated data contain SDFs calculated using TSUNAMI-3D with KENO as the transport solver and TSUNAMI-1D using XSDRN as the transport solver. The SDFs obtained with each of these transport methods are located in subfolders bearing those names. The SDFs provided by ORNL are formatted as .zip files and are extractable with either the `unzip` function in Linux or the standard Windows Explorer feature. The NEA SDFs are organized in subdirectories the fissile species, e.g., *HEU* [highly enriched uranium] or PU [plutonium]. The NEA SDFs are stored as .gz files which can be unzipped using the gunzip command in the Linux operating system or by using a variety of commercially available utilities (WinZip, 7zip) in Windows. It is noted that there is some overlap in the ORNL- and NEA-generated SDFs.

SCALE Usage Experience with ICSBEP SDFs by Source

The ORNL SDFs contain 464 SDFs generated using TSUNAMI-3D and 80 SDFs generated using TSUNAMI-1D. All calculations were performed using SCALE 6.0. These files are all known to be compatible with the TSUNAMI-IP module.

The SDFs from NEA were generated using a variety of methods and have differing resulting formats. At present, not all of these formats are supported by TSUNAMI-IP. The NEA-generated SDFs, which were produced with MCNP, are not readable by TSUNAMI-IP at this time. These SDFs are recognizable because they contain *MCNP* in the filenames. Additionally, files generated using MKK KENO are also not readable with TSUNAMI-IP. According to the readme file associated with the NEA SDFs, there were 368 cases which added P1 elastic scattering sensitivity coefficients. These cases are distributed among the HEU-SOL-THERM, HEU-MET-FAST, and PU-MET-FAST experimental categories. These cases are partially readable by TSUNAMI-IP. While the TSUNAMI-IP calculations do not result in a failed computer run, there are several important sensitivities that are apparently not considered in the calculation. A calculated $\boldsymbol{c_k}$ value near zero is evidence that one of these SDFs has been inadvertently included in a calculation. The files containing this information can be identified using the "grep" function of the Linux operating system using the following command.

```
grep "elastic-P1" list_of_file_names
```

Applicability of SDFs

Users frequently ask how the SDFs distributed with the ICSBEP Handbook can be used. This section addresses that question, although there is not currently a clear consensus answer beyond ORNL.

The SDFs distributed with the ICSBEP Handbook can be used to screen critical experiments against the application for similarity. Historically, criticality analysts have used physical parameters such as enrichment, the ratio of moderating species to fissioning species, or some measure of the neutron energy spectrum to establish applicability of an experiment to the validation of a particular application. Typically, analysts compare these values to published values in the ICSBEP Handbook and determine whether they are sufficiently close to warrant inclusion in a validation suite. The SDFs from the ICSBEP Handbook to calculate $\boldsymbol{c_k}$ values with the application case is fulfilling the same purpose in that the analyst is comparing nonquality assured values from the Handbook to determine whether an application should be included in a validation effort or not.

Further use of the SDFs from the ICSBEP Handbook— such as using the $\boldsymbol{c_k}$ values as a trending parameter for bias assessment or using the SDFs in a data adjustment calculation— would require that the SDFs be checked against direct perturbation calculations. It is also noted that the k_{eff} values reported in the TSUNAMI-IP calculations would not apply to validation due to the variety of computational methods used to generate the SDFs. However, this can easily be supplemented with k_{eff} values calculated by each analyst using the appropriate methodology. The sensitivities do not change dramatically with different cross section libraries, so the similarity assessment between the application and experiments is unaffected by the variety of cross section libraries used in the generation of the ICSBEP Handbook SDFs. This was demonstrated in sensitivity studies using ENDF/B-V and ENDF/B-VI in NUREG/CR-7109 [6].

Use of File Injection in SCALE Inputs

One of the more onerous tasks of assembling TSUNAMI-IP input to screen critical experiments against the application of interest is entering a large number of file paths and names. It is often convenient to set up a single file or files containing the input necessary for the SDFs that could prove useful across multiple applications. A seldom-discussed capability that has been available since SCALE 6.0, known as *file injection*, allows for the wholesale inclusion of an entire file within a SCALE input during execution.

File injection is a convenient way to include a list of SDFs in the shell and the experiment blocks of the input. To inject a file into SCALE input during execution, the user simply indicates the action using the < arrow. An example is included below for a case in which a user has set up a file named "exps.dat" containing the list of experiments to be included in the experiments block of a TSUNAMI-IP input.

```
read exps
< /path_to_my_base_directory/experiments/exps.dat
end exps
```

Logistics of Injecting ICSBEP Handbook SDFs

Useful files must be created to take advantage of SCALE's file injection capability. At ORNL, these files are generally created on Linux computing clusters using command line scripts and commands. Other options,

including python or perl scripts or small FORTRAN programs, can also be used effectively. A command line process is presented briefly below to help users create these files quickly.

The distributed SDFs must be copied from the ICSBEP Handbook to the compute cluster and unzipped in disk space that is available to the user during execution. The SDFs will be linked from that location to the SCALE temporary directory so they can be used in the TSUNAMI-IP calculations. The "`ls -l`" command provides a list of all files in the current directory in a single column. The output from this command can be sent to awk via pipe and printed twice, preceded by "`ln -s`" to create the symbolic link. Lastly, the output should be redirected to the file that will ultimately be inserted into the TSUNAMI-IP input. An example of the entire command for the intermediate enrichment (IEU) SDFs is as follows:

```
> ls -1 IEU* | awk '{print "ln -s "$1, $1}' > shell.file
```

The first line of the result of this execution for the IEU-SOL-THERM-001 SDFs is:

```
> ln -s IEU-SOL-THERM-001-001_KENO_ENDF-B-VII.0---238-
Group_SENS IEU-SOL-THERM-001-001_KENO_ENDF-B-VII.0---238-
Group_SENS
```

The path to the SDF still must be added immediately prior to the first instance of the filename. This can be accomplished by making a sed modification to the file created in the previous step. This can be difficult because each forward slash in the directory structure must be escaped with a backslash. The sed command could look like the line shown here:

```
> sed -i 's/-s /-s \/projects\/NEA_SDF\/IEU\/testing\//'
shell.file
```

The first line of the resulting file would be as follows:

```
> ln -s /projects/NEA_SDF/IEU/testing/IEU-SOL-THERM-001-
001_KENO_ENDF-B-VII.0---238-Group_SENS IEU-SOL-THERM-001-
001_KENO_ENDF-B-VII.0---238-Group_SENS
```

The next step is to add "`=shell`" on line 1 and an "end" on the last line of this file. This is typically accomplished with a text editor.

The second file needed is a single list of all the SDFs to be injected into the experiments block. This file is much easier to generate and can be created by redirecting the list (e.g., `ls -1 IEU*`) to a file. The final step in creating the shell sequence file, called shell.file here, is to add a link to the file listing the SDFs for the experiments block. This is also typically achieved in a text editor since it is a single line addition.

Alternatively, the entire path to the list of SDFs can be provided in the injection statement in the TSUNAMI-IP input. The advantage to linking this file is that it can be linked to a generic name, and then multiple TSUNAMI-IP inputs can be generated, with changes needed only in the shell block. Because file paths in the experiments block are currently limited to 80 characters in TSUNAMI-IP, the files can be linked via the shell block to circumvent this limitation.

CONCLUSION

A primary barrier to the implementation of S/U methods in criticality safety validation is the engineering and computation time necessary to generate an appropriate library of SDFs for a large number of critical experiments. ORNL has worked to ameliorate this difficulty by distributing over 450 SDFs generated through the VALID procedure. The NEA has also generated and made available several thousand additional SDFs. These files can be used directly by analysts to screen experiments for applicability to specific safety application models. The confirmation of the sensitivity data with direct perturbation calculations [7] should allow somewhat broader application of these data for trending on the c_k parameter and estimating penalty factors for unvalidated nuclides. None of these data can eliminate the requirement that each institution must generate its own models and k_{eff} values for use in validation, but the process of implementing rigorous, modern S/U-based validation techniques can be streamlined by using this available resource.

ACKNOWLEDGMENTS

The preparation and presentation of this paper were supported by the US Department of Energy Nuclear Criticality Safety Program.

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