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Development and testing of WEASEL for least-squares neutron spectrum adjustment

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Abstract. A new least-squares adjustment program called WEASEL has been developed. WEASEL is implemented in Python and uses standard ASCII interfaces for user input and output, and HDF5 interfaces for cross section, covariance data, and weighting function data. WEASEL allows the user to supply a trial neutron spectrum in an arbitrary group structure. The trial neutron spectrum is re-binned into a group structure consistent with the covariance data using a weighting function that can either be read from the data library or supplied as input by the user. WEASEL performs least-squares adjustments of a single irradiation environment. The adjusted neutron spectrum, covariance matrices, and other derived quantities can then be plotted and interrogated with standard software packages.

1 Introduction

Westinghouse has performed least-squares adjustment of neutron spectra for many years using modified versions of SAND [1] and FERRET [2]. SAND is used to re-bin an input trial spectrum to a 53-energy group format, and FERRET performs the least-squares reconciliation of the trial spectrum, the reactor dosimetry measurements, and the dosimetry cross sections with their respective uncertainties.

SAND and FERRET were brought into Westinghouse in the 1970s and underwent additional proprietary development since that time. Use of this software has raised questions in recent years about ownership and licensing obligations. Further, due to the age of the software, rigorous documentation of its design and validation basis is not readily available. The software is written in a legacy dialect of Fortran that is difficult to understand and maintain for current engineers, and it suffers from limitations in the size of problems that it can address, which prevents it from being benchmarked against similar software.

To overcome these problems, a new program called WEASEL has been developed. WEASEL is heavily inspired by work done by Williams, et. al. on NSVA-3 [3]. This paper describes the code, the equations solved, and provides results of benchmarking exercises that demonstrate that the code successfully overcomes the limitations associated with SAND and FERRET and is suitable for use in future reactor dosimetry evaluations.

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2 Methodology

2.1 Spectrum Re-Binning

The first step of the spectrum adjustment process employed by Westinghouse involves re-binning the input trial spectrum, typically supplied in the 47-group BUGLE-96 energy group structure, to the energy grid associated with the dosimetry cross sections. Currently, the Westinghouse version of the SNLRML dosimetry library [4] uses a 53-group structure. The Westinghouse version of the SAND code performs this re-binning operation using a cubic spline on a log-log grid to re-construct a continuous shape between the user-supplied data points. At low and high energies, simple fitting functions are assumed.

For the WEASEL code, it was decided that a better approach would be to use the results of a transport calculation performed on a more refined energy grid for a representative geometry. This "fine-group" weighting function is used to represent the shape of the neutron spectrum within each trial energy group supplied by the user. With this information, user-supplied trial spectra in any group structure can be accurately re-binned into the group structure of the dosimetry cross sections. Fig. 1 shows weighting spectra developed using the VITAMIN-B6 library [5] for LWR irradiations.

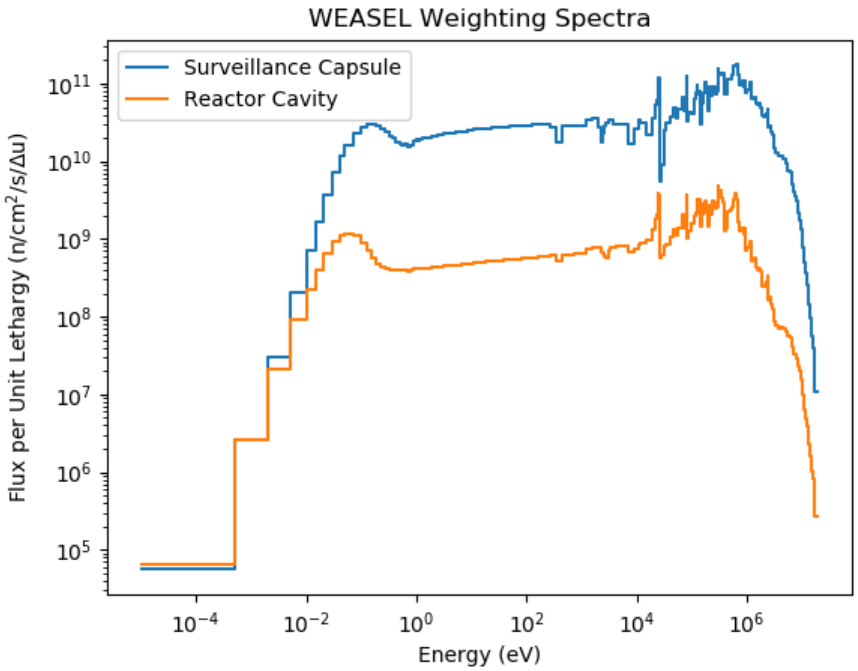

Fig. 1. Weighting neutron spectra included in the WEASEL SNLRML library.

2.2 Flux Covariance

WEASEL can compute a relative flux covariance matrix from the following relationship:

$$M_{gg'} = R_{NORM}^2 + R_g * R_{g'} * P_{gg'} \quad (1)$$

where R_{NORM} specifies an overall fractional normalization uncertainty, and the fractional uncertainties $R_{g\prime}$ and R_g specify additional random groupwise uncertainties that are correlated with a correlation matrix given by:

$$P_{gg\prime} = [1 - \theta]\delta_{gg\prime} + \theta e^{-H} \tag{2}$$

where

$$H = \frac{(g - g')^2}{2\gamma^2} \tag{3}$$

The first term in the correlation matrix equation specifies purely random uncertainties, while the second term describes the short-range correlations over a group range γ (θ specifies the strength of the latter term). The value of δ is 1.0 when g = g′ and 0.0 otherwise. The same method is employed in the Westinghouse FERRET code. Typical values for these parameters are given in the WCAP-18124-NP-A [6].

2.3 Flux Adjustment

WEASEL computes the adjusted flux using the same equations as the NSVA-3 computer code [3]. Consider a neutron spectrum with g energy groups and a set of dosimetry measurements from n reactions. The sensitivity matrix of the flux (size: g rows by n columns) is defined as the concatenation of the reaction cross sections, σ_n, for each of the n reactions being used for the least-squares fitting:

$$S_\phi = [\sigma_1\ \sigma_2\ \sigma_3\ \cdots\ \sigma_n] \tag{4}$$

The sensitivity matrix of the cross sections (size: n rows and $n \times g$ columns) is defined as:

$$S_\sigma = \begin{bmatrix} \phi^{\mathrm{T}} & 0 & \cdots & 0 \\ 0 & \phi^{\mathrm{T}} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \phi^{\mathrm{T}} \end{bmatrix} \tag{5}$$

In the equation above, ϕ is the trial flux spectrum. Finally, the block covariance matrix (size: $n \times g$ rows by $n \times g$ columns) is defined as:

$$\mathrm{Cov}_{\sigma_{1\ldots n}} = \begin{bmatrix} \mathrm{Cov}_{\sigma_1} & 0 & \cdots & 0 \\ 0 & \mathrm{Cov}_{\sigma_2} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \mathrm{Cov}_{\sigma_n} \end{bmatrix} \tag{6}$$

The matrix, h, is defined as:

$$h = S_\phi\ \mathrm{Cov}_\phi\ {S_\phi}^{\mathrm{T}} + S_\sigma\ \mathrm{Cov}_{\sigma_{1\ldots n}}\ {S_\sigma}^{\mathrm{T}} + \mathrm{Cov}_{R_m} \tag{7}$$

WEASEL computes the adjusted (best-estimate) flux, ϕ_A, as:

$$\phi_A = \phi_{WEASEL} + \mathrm{Cov}_\phi\ S_\phi\ h^{-1}\ (R_m - R_c) \tag{8}$$

R_m and R_c are the measured and calculated reaction rates, respectively. The adjusted (best-estimate) flux covariance matrix, Cov_{ϕ_A}, is:

$$\mathrm{Cov}_{\phi_A} = \mathrm{Cov}_\phi - \mathrm{Cov}_\phi\ S_\phi\ h^{-1}\ \left({S_\phi}^{\mathrm{T}}\ \mathrm{Cov}_\phi\right) \tag{9}$$

3 Implementation

WEASEL is implemented in Python Version 3 with dependencies on widely-used third-party modules: Numpy, Scipy, and h5py. The total implementation, including all input parsing, error checking, and output formatting, requires slightly more than 1000 lines of code.

Input consists of a simple flat text file. Matrices and arrays can be directly copied and pasted from spreadsheets with no formatting changes required. The user can supply measured reaction rates and uncertainties, as well as an optional correlation matrix for the measurement data. Reaction rates can be adjusted for the presence of cover materials. The user must also supply a prior ("trial") flux spectrum, as well as the associated energy group boundaries and a weighting spectrum for the re-binning operation. (If no re-binning is needed, a flat weighing spectrum can be employed.) The prior flux covariance matrix can be calculated according to Equation (1) or supplied directly by the user.

Outputs include standard ASCII printouts and comprehensive results of the calculation embedded in an HDF5 file. The HDF5 file can be readily post-processed to generate plots to visualize the results. See Fig. 2 and Fig. 3, for example.

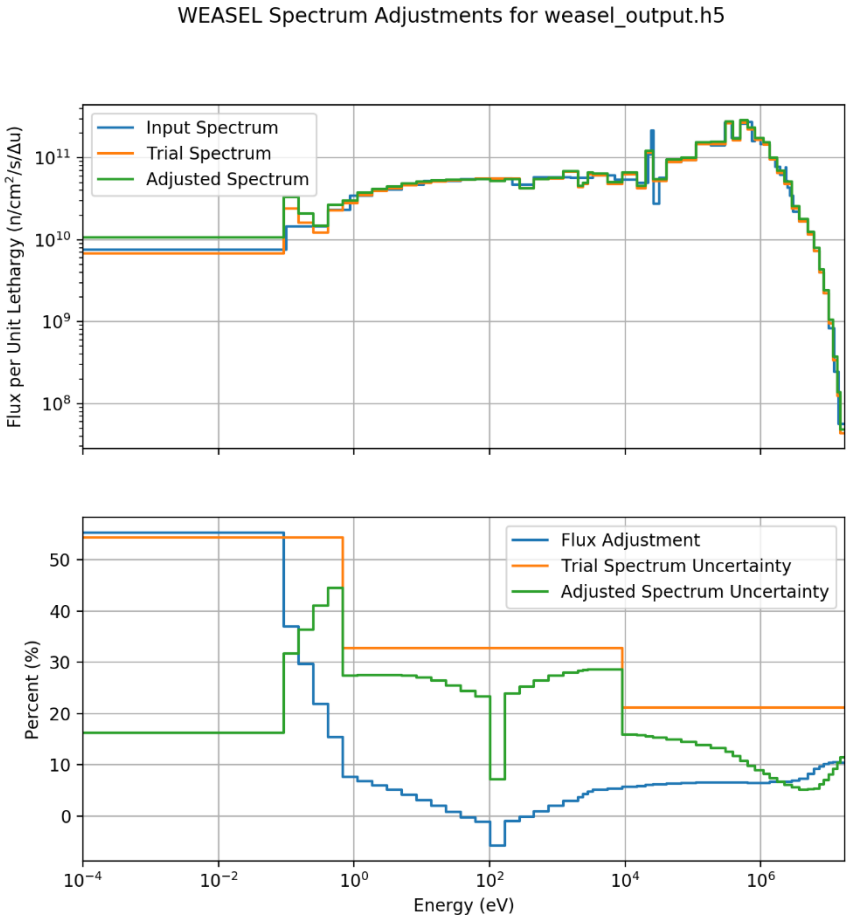

Fig. 2. Typical neutron spectra plot from the HDF5 output file produced by WEASEL.

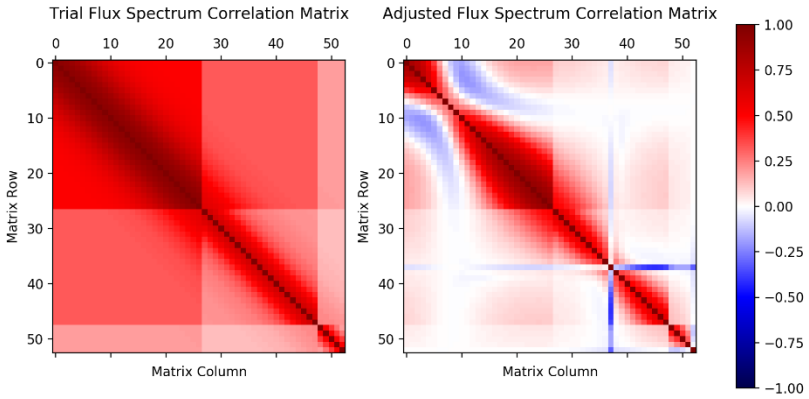

Fig. 3. Typical correlation matrices plot from the HDF5 output file produced by WEASEL.

4 Benchmarking

4.1 In-Vessel Surveillance Capsule

To compare results generated by WEASEL to results from SAND and FERRET, a typical surveillance capsule from a Westinghouse 4-Loop reactor was evaluated with both codes. The tests used IRDFF-II [7] dosimetry cross section and covariance data sets.

Comparisons of WEASEL and SFI results for the surveillance capsule appear in Table 1 through Table 3. Results from Table 1 through Table 3 show good agreement. The reaction rates for the high-energy threshold reactions are very consistent, with somewhat larger differences observed in the reaction rates sensitive to low energy neutrons. Note that SAND's method for re-binning the trial neutron spectrum in the thermal energy range is crude. WEASEL's method makes better assumptions about the shape of the neutron spectrum in the thermal energy range, derived from fine-group transport calculations.

Table 1. Comparison of best-estimate reaction rates for the in-vessel surveillance capsule.

Reaction	WEASEL Reaction Rate (rps/atom)	SAND-FERRET Reaction Rate (rps/atom)	WEASEL / SAND-FERRET
Cu-63 (n,a) Co-60	5.87E-17	5.90E-17	0.995
Fe-54 (n,p) Mn-54	6.48E-15	6.47E-15	1.002
Ni-58 (n,p) Co-58	9.32E-15	9.32E-15	1.000
Co-59 (n,g) Co-60	6.26E-12	6.34E-12	0.987
Co-59 (n,g) Co-60*	3.66E-12	3.63E-12	1.008
U-238 (n,f) fp*	3.82E-14	3.84E-14	0.995
Np-237 (n,f) fp*	4.22E-13	4.23E-13	0.998

Table 2. Comparison of best-estimate response rates for the in-vessel surveillance capsule.

Reaction	WEASEL Response	SAND-FERRET Response	WEASEL / SAND-FERRET
Flux, E> 1.0 MeV	1.20E+11	1.21E+11	0.994
Flux, E> 0.1 MeV	5.65E+11	5.66E+11	0.999
Flux, E< 0.414 eV	1.12E+11	1.01E+11	1.104
dpa/second	2.38E-10	2.45E-10	0.969
Flux, E> 0.0 MeV	1.36E+12	1.34E+12	1.014

Table 3. Comparison of best-estimate response rate uncertainty for the in-vessel surveillance capsule.

Reaction	WEASEL Uncertainty (%)	SAND-FERRET Uncertainty (%)
Flux, E> 1.0 MeV	5	6
Flux, E> 0.1 MeV	9	9
Flux, E< 0.414 eV	13	13
dpa/second	7	7
Flux, E> 0.0 MeV	8	8

4.2 Comparisons to NSVA-3

To validate the overall implementation of the method, results produced by WEASEL were compared to results produced by the NSVA-3 for the analysis of an irradiation performed at the Sandia Pulsed Reactor (SPR) and described in [8]. This test case is included as an example problem with the NSVA-3 code and employs dosimetry cross section data form the SNLRML library in an 89-group format. Data from this irradiation included 26 reactions; the SAND-FERRET sequence is unable to perform this analysis due to array dimensioning limitations embedded in SAND and FERRET.

The adjusted spectra, adjusted reaction rates, and associated uncertainties produced by NSVA-3 and WEASEL are nearly identical, differing by no more than 0.03%.

5 Conclusion

WEASEL provides a modern, flexible, user-friendly means of performing least-squares neutron spectrum adjustments. The theoretical basis of the code has been comprehensively documented and the software implementation has been rigorously validated. It is suitable for use as a replacement for the SAND and FERRET computer codes.

Thanks to John Williams for sharing the NSVA-3 computer code and for his generous assistance with questions along the way.

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