Sensitivity and Uncertainty Analysis
Tools Used at the Jožef Stefan Institute

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3D sensitivity / uncertainty analysis
codes and data

Cross section sensitivity, uncertainty and adjustment tools

- **GANDR (data library, ZOTT, SEMOVE)** - Sensitivity-Based Global Assessment of Nuclear Data Requirements
- **SUSD3D**: 1D, 2D, 3D SN uncertainty including SED/SAD; coupled to transport codes DOORS, DANTSYS, extension to PARTISN, DRAGON etc. planned.
- **ANGELO-LAMBDA** with the corresponding library **ZZ-SCALE6.0/ COVA-44G**: utility programs for interpolating or collapsing and mathematical verification of the 44-group covariances available in SCALE-5.1 and 6.0. Work carried out within the Expert Group on Uncertainty Analysis in Modelling (UAM).
- **Covariance data produced by GANDR** (IAEA evaluations for Th, W)
GANDR - Sensitivity-Based Global Assessment of Nuclear Data Requirements

• Technical leader: D. W. Muir
• Computerized planning tool for nuclear data development, to **assess the impact of new experimental information on evaluated cross sections and integral parameters.** It is capable of ranking competing proposals for new nuclear data measurements.
• Based on sensitivity and uncertainty analysis
• Linked to EXFOR differential measurement database and integral benchmark databases (**SINBAD, IRPhE, ICSBEP**)
• **Global evaluation of data covariances, taking into account of all high-quality differential and clean integral data.**
• **SEMOVE, A Computer Program for Calculating Derivatives of Processed Multigroup Nuclear Data by Discrete Differences**
• **ZOTTVL, Data Evaluation Using Partitioned Least-Squares**
• [http://www-nds.iaea.org/gandr](http://www-nds.iaea.org/gandr)
IAEA1371: ZOTT99, Data Evaluation Using Partitioned Least-Squares (D.W. Muir)

• The method of solution is partitioned least squares, which is a form of minimum variance linear estimation (least squares) featuring reduced matrix-inversion requirements (relative to methods based on solving the conventional normal equations). Partitioned least squares permits general correlations among all data uncertainties, including cross-type correlations between differential and integral data. If the problem to be solved is precisely linear, and if correct input is supplied by the user, then the minimum-variance solution obtained with ZOTT99 is unique and exact. At user request, the code will perform a minimally invasive modification of the input covariance matrix to enforce consistency (unit chi-squared). Only the diagonal elements are changed, and an iterative procedure is followed in which only one diagonal element is changed at a time, namely, the one which produces the maximum benefit in lowering chi-squared. This process is repeated until chi-squared reaches unity.

SEMOVE/GANDR is a Fortran-77 computer program for computing the derivatives of processed multigroup nuclear data with respect to the individual parameters of the GANDR library. The basic premise is that a user has chosen a multigroup processing program such as NJOY and has developed a script that allows the calculation of all nuclear data of interest in his selected group structure and with his selected weight function. A distinctive feature of the GANDR project is that the fundamental data uncertainties are assumed to reside, not in the ENDF evaluations, but in the parameters of the GANDR library.

To interface the GANDR library with normal sensitivity tools (such as SUSD3D), and thereby to permit the GANDR library to be improved by exploiting the information content of accurate integral data, SEMOVE calculates the changes in the multigroup cross sections that result from changes in the GANDR parameters.
GANDR - Sensitivity-Based Global Assessment of Nuclear Data Requirements - Planned Extensions

- Self-shielded cross sections: development of methods for the calculation of the sensitivity of "pseudo-composition-independent" self-shielded multigroup cross sections to the pointwise parameters of the GANDR evaluation system. Such self-shielded cross sections are parameterized by particular values of the "background" cross section sigma-zero. In defining these cross sections, the Bondarenko flux model should be employed.

- Development of methods for the calculation of the sensitivity to angular distributions, such as the P-1 component of elastic and inelastic scattering, to the pointwise parameters of the GANDR evaluation system.

- Develop the discrete-difference approach to the calculation of the GANDR parameter sensitivity matrix R. Apply the method to a problem that includes significant resonance self-shielding, such as a critical assembly. Compare the effect on adjusted GANDR.
NEA-1628: SUSD3D, A Multi-Dimensional, Discrete Ordinates Based Cross-Section Sensitivity & Uncertainty Code

SUSD3D calculates sensitivity coefficients and standard deviation in the calculated detector responses or design parameters of interest due to input cross sections and their uncertainties. First-order perturbation theory is used. One-, two- and three-dimensional transport problems can be studied.

Several types of uncertainties can be considered, i.e. those due to:
(1) neutron/gamma multigroup cross sections,
(2) energy-dependent response functions,
(3) secondary angular distribution (SAD) or secondary energy distribution (SED) uncertainties.

SUSD3D can use the flux moment or angular flux files produced by the ANISN, DORT, TORT, ONEDANT, TWODANT and THREEDANT discrete ordinates codes.
- Runs on PC-DOS, LINUX, UNIX, etc.
SUSD3D sensitivity & uncertainty code system

Main features

• Suitable for complex 1D, 2D and 3D sensitivity-uncertainty analysis.
• Reduced memory requirement
• SAD/SED effects
• Runs on PC (DOS, LINUX), UNIX
• Fortran-95
• New plotting tools were developed
• Variable mesh option (TORT), first collision source

Φ, Φ⁺
Partial X-sections
Group covariances
Group SAD/SED covariances

DOORS DANTSYS DRAGON
GROUPR GROUPSR ANGELO ERRORR ERRORR34

SUSD3D
SUSD3D code - recent updates

- Code was rewritten from F77 to F95 (updated memory, data management, language level).
- Fission spectra uncertainties can be calculated using the file MF35 data processed by the ERRORR code. Re-normalisation of the prompt fission spectra covariance matrices can be applied using the *constrained sensitivity method*. This option is useful in case if the fission spectra covariances do not comply with the ENDF-6 Format Manual rules. In this way SCALE6 fission spectra covariances processed by ANGELO code can be used in SUSD3D directly (collapsing would otherwise be wrong as it does not preserve the normalisation).
- Cross sections can be input directly on input card "xs".
- For $k$-eff analysis the normalisation of the sensitivity profiles is done internally.
- Calculation of absolute sensitivities for SEMOVE/GANDR

**Ongoing:**
- Pre- and post-processing (interfaces with DICE-PLOT (Soppera Nicolas, Manuel Bossant) & PLOT-S (Slavko Slavic) plotting utilities
- Self-shielding treatment improvements
- Methodology for 3D analysis (1st collision source and hybrid methods)
- Extension to other codes (PARTISN, DRAGON …)
Examples of SUSD3D Analysis

- **Reactor pressure vessel surveillance dosimetry**: uncertainty in predicted dosimeter reaction rates and PV exposition, determination of safety margins --> reactor lifetime predictions (ANISN, TWODANT)

- **Fission shielding benchmarks**:  
  - ASPIS (ANISN, TWODANT),  
  - VENUS-3 (TORT)

- **Fusion benchmarks**: preparation & post-analysis (GRTUNCL/DORT-TORT) :  
  - FNG Bulk Shield benchmark,  
  - FNG Streaming,  
  - FNG SiC,  
  - FNG Tungsten,  
  - FNG-HCPB tritium breeding benchmark,  
  - FNG-HCLL tritium breeding benchmark;

- **Criticality benchmarks**: (TWODANT, THREEDANT)  
  - KRITZ-2,  
  - SNEAK-7  
  - VENUS-2

- **Oil well logging**: C/O (gamma) ratio sensitivity & uncertainty (DORT)

- **QUADOS - TLD response function**: (ANISN)

- **Discrete Ordinates vs. M/C sensitivity method validation**: (Iron shell TOF benchmark, MCSEN/SUSD3D/SUSD-FNS analysis, SAD sensitivities)
Cross-Section Covariance Matrices
Data Formats for Cross Section Covariances in Evaluated Files

Processing available (NJOY/ERRORR)

- **MF=31**: covariance of average number of neutrons per fission ($\nu$ - MT=452, 455, 456)
- **MF=32**: Shape and area of individual resonances
- **MF=33**: covariance of neutron cross section
- **MF=34**: covariance of angular distribution of secondary neutron (MT=2/P1 only)
- **MF=35**: covariance of energy distribution of secondary neutron (MT=18 only)

No processing available:

- **MF=30**: Covariances obtained from parameter covariances and sensitivities
- **MF=40**: Covariances for production of radioactive nuclei
MF=34 (Covariance of $\bar{\mu}$)

$\bar{\mu}$: average cosine of the scattering angle for elastic

- MF=3/MT=251: $\mu$ (multigroup constants in LAB)
- MF=3/MT=2: elastic scattering cross sections
- MF=4/MT=2: angular distributions for elastic scattering – CM
- MF=34/MT=2: covariance of P1 Legendre component – CM (LAB)

In JENDL-3.3 evaluations the covariances of $\mu$ are given in MF=34 in CM system, and are converted by ERRORJ to LAB.

PROBLEM:
- Loss of accuracy in CM $\rightarrow$ LAB transformation.

Recommendation:
- Add in ERRORJ processing of covariances into CM
- Modify ERRORJ to allow the LAB representation of covariance of $\mu$ in MF=34. No need for conversion.
MF=35 (Covariance of $\chi$)

- Fission spectra covariances data without scaling by the bin-energy widths. **In this way it is numerically easier to fulfil the requirement that the rows and columns of the matrices must sum to 0.**
- **Verification procedure needed** to check that the rows & columns sum to 0 ($<10^{-5}$).
Available Cross-Section Covariance Data

**ENDF/B-V (MF 31, 32, 33)**

**ENDF/B-VI.8 (MF 31, 32, 33)**

**ENDF/B-VII.0 (MF 31, 32, 33)**

**JEFF-3.0 (MF 31, 33)**

**JENDL-3.3 (MF 31, 32, 33, 34, 35)**

**IRDF-2002 (MF 33)**

**TENDL-2008 (MF 32, 33, 34)**
- 348 isotopes, 267 stable and 81 radioactive (from F-19 to Bi-210)
Processing Codes and Multigroup Covariance Data Libraries (cont.)

- **NJOY-99/ERRORR**: MF=31-35 processing code; new fission spectra covariance (MF35) processing was updated (Trkov)
- **PUFF-IV**: Code System to Generate Multigroup Covariance Matrices from ENDF/B-VI Uncertainty Files (COVERX Format)
- **ANGELO-LAMBDA** with the corresponding libraries **ZZ-SCALE5.1/ZZ-SCALE6/COVA-44G**: utility programs for interpolation and mathematical verification of the matrices was extended to handle the 44-group covariances available in SCALE-6. Work carried out within the Expert Group on Uncertainty Analysis in Modelling (UAM).
ZZ-SCALE6/COVA-44G, 44-group cross section covariance matrix library extracted from SCALE6


• The SCALE6 covariance library data correspond to 44-group relative uncertainties assembled from a variety of sources, including evaluations from ENDF/B-VII, ENDF/B-VI, JENDL-3.3, and more than 300 approximated uncertainties from a collaborative project performed by Brookhaven National Laboratory (BNL), Los Alamos National Laboratory (LANL), and Oak Ridge National Laboratory (ORNL). The current SCALE covariance library spans the full energy range of the multigroup cross-section libraries, while the approximate uncertainty data in SCALE 5.1 did not extend above 5 keV. More than 100 new materials have also been added to the covariance library.

• it is assumed that the same relative (rather than absolute) uncertainties can be applied to all cross-section libraries, even if these are not strictly consistent with the nuclear data evaluations.
  – The library includes evaluated covariances obtained from ENDF/B-VII, ENDF/B-VI, and JENDL3.3 for more than 50 materials
  – reactions or parameters: total, elastic, inelastic, (n,2n), fission, $\chi$, (n,$\gamma$), (n,p), (n,d), (n,t), (n,h), (n,$\alpha$), $\nu$
**ZZ-SCALE6/COVA-44G, 44-group cross section covariance matrix library extracted from SCALE6**

- Among the materials in the SCALE library with covariances taken from high-fidelity nuclear data evaluations are the following:
  
  (a) ENDF/B-VII evaluations (*includes both VII.0 and pre-release covariances proposed for VII.1*): \(\text{Au, } ^{209}\text{Bi, } ^{59}\text{Co, } ^{152,154,155,156}\text{Gd, } ^{191,193}\text{I, } ^{7}\text{Li, } ^{23}\text{Na, } ^{93}\text{Nb, } ^{58}\text{Ni, } ^{99}\text{Tc, } ^{232}\text{Th, } ^{48}\text{Ti, } ^{239}\text{Pu, } ^{233,235,238}\text{U, } \text{V}\)
  
  (b) ENDF/B-VI evaluations: \(\text{Al, } ^{241}\text{Am, } ^{10}\text{B, } ^{12}\text{C, } ^{50,52,53,54}\text{Cr, } ^{63,65}\text{Cu, } ^{54,56,57}\text{Fe, } ^{55}\text{Mn, } ^{60,61,62,64}\text{Ni, } ^{206,207,208}\text{Pb, } ^{242}\text{Pu, } ^{28,29}\text{Si}\)
  
  (c) JENDL-3.3 evaluations: \(\text{ } ^{11}\text{B, } ^{1}\text{H, } ^{16}\text{O, } ^{240,241}\text{Pu}\)

- At the other end of the spectrum from high fidelity data, “low-fidelity” (lo-fi) covariances (BLO data) are defined to be those that are estimated independently of a specific data evaluation. The approximate covariance data in SCALE are based on results from a collaborative project funded by the Department of Energy Nuclear Criticality Safety Program to generate lo-fi covariances over the energy range from 10-5 eV to 20 MeV for materials without covariances in ENDF/B-VII.0. Nuclear data experts at BNL, LANL, and ORNL devised simple procedures to estimate data uncertainties in the absence of high fidelity covariance evaluations. The result of this project is a set of covariance data in ENDF/B file 33 format that can be processed into multigroup covariances.
Nuclides with covariance data in ZZ-SCALE6/COVA-44G

ANGELO/LAMBDA codes and Covariance Matrix Libraries

Content of the libraries:

• Covariance matrices:
  - library format: BOXER or COVERX;
  - energy group structure: arbitrary (usually same as in evaluated files).

• ANGEL02.3 code for interpolation of covariance matrices to user defined energy group structure; only file-33 covariance matrices can be treated. (Cross-correlation between reactions are treated correctly but not cross-correlations between nuclides)

ADVANTAGES: easy to use & fast alternative to NJOY processing
DISADVANTAGES: no flux or cross-section weighting

NOTE: processing of fission spectra covariances by ANGEL0 code may not preserve the normalisation of the matrix (zero-sum rule), therefore the use of constrained sensitivity method as coded in SAGEP and SUSD3D is mandatory to determine the corresponding uncertainties.

• LAMBDA2.3 code for verification of mathematical properties of covariance matrices.
## Fission spectra induced uncertainty

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<th>Uncertainty [pcm]</th>
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<td>Exact</td>
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<td>KRITZ2.19H (18g)</td>
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<td>SNEAK-7A (80g)</td>
<td>283.6</td>
<td>247.5</td>
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<tr>
<td>SNEAK-7B (80g)</td>
<td>347.6</td>
<td>315.2</td>
<td>319.1</td>
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KRITZ-2 Benchmarks : C/ E in $k_{\text{eff}}$ (in pcm), compared with the experimental and computational uncertainties

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<tr>
<td>(C/E-1) JEFF3.1</td>
<td>-500</td>
<td>-430</td>
<td>-160</td>
<td>-370</td>
<td>-530</td>
<td>-440</td>
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<tr>
<td>(C/E-1) ENDF/B-VII</td>
<td>-330</td>
<td>0</td>
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<td>Experimental &amp; model uncertainty</td>
<td>180</td>
<td>260</td>
<td>210</td>
<td>200</td>
<td>270</td>
<td>250</td>
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<tr>
<td>XS uncertainty (JENDL-3.3)</td>
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<td>590</td>
<td>490</td>
<td>530</td>
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<td>2000</td>
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<td>640</td>
<td>560</td>
<td>590</td>
<td>790</td>
<td>770</td>
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Model test case:
- high C/E differences
- covariances available including MF34
- deterministic and MC models available

Differences between predicted and measured keff (in pcm) using ENDF/B-VII and new IAEA W evaluation.
CONCLUSIONS

• Sensitivity and uncertainty system composed of tools which are all available in public domain.

• Study of ZPR-9 case is suitable for method performance and model tests because of high C/E discrepancies and availability of needed information (computational model, covariance data).
3D sensitivity / uncertainty analysis: projects

- **Uncertainty Analysis in Modeling (UAM):** elaborate a state-of-the-art report on current status and needs of sensitivity and uncertainty (SU) analysis in modeling, with emphasis on multi-physics (coupled) and multi-scale simulations. The objective is to determine the uncertainty in LWR system calculations at all stages of coupled reactor physics/thermal hydraulics calculation. The full chain of uncertainty propagation from basic data, engineering uncertainties, across different scales (multi-scale), and physics phenomena (multi-physics) is tested on a number of benchmark exercises for which experimental data is available and for which the power plant details have been released;

- A **sensitivity and uncertainty benchmark** based on the SNEAK experiments will be launched in co-ordination with Expert Group on WPRS-UAM and IRPhE to compare the performances of different computer tools available;

- **European Fusion File (EFF) activity** (**SINBAD**, benchmark SU analysis, cross section validation);

- **ANDES**, Accurate Nuclear Data for Nuclear Energy Sustainability.