SUSD3D, A MULTI-DIMENSIONAL, DISCRETE ORDINATES BASED CROSS SECTION SENSITIVITY AND UNCERTAINTY CODE

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ABSTRACT

1. **Program Name and Title:** SUSD3D: One-, Two- and Three-Dimensional Cross Section Sensitivity and Uncertainty Code.

2. **Computer for Which Program is Designed and Other Machine Versions Available:** SUSD3D was used on personal computer, VAX, and HP Workstation.

3. **Problem Solved:** 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. 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 development was started from the SUSD [6] code. Besides several minor modifications and extensions SUSD3D differs from SUSD in particular that:
   - Three-dimensional analysis is possible,
   - Flux moment files are used to evaluate the sensitivity profiles, instead of angular flux files; substantially reducing in this was the computer space requirements. SUSD3D can use the flux moment files produced by the DORT, TORT [7], ONEDANT, TWODANT and THREEDANT [8] discrete ordinates codes. The method used in the SUSD code based on the angular flux files from the ANISN [9] and DOT-III codes was kept for comparison,
   - Processing codes were updated to the ENDF-6 format,
   - Processing of SAD covariance matrices was programmed,
   - Complete SAD covariance matrices can be taken into account in SUSD3D to calculate the variance.

4. **Method of Solution:** First-order perturbation theory is used to obtain sensitivity coefficients. They are derived from the direct and adjoint flux moments (or angular fluxes) calculated by the discrete ordinates codes listed above. The sensitivity profiles are folded

with the cross section covariance matrices to determine the variance and standard deviation in an integral response of interest.

5. **Restrictions on the Complexity of the Problem:** Variable dimensioning is used providing flexibility to adjust the storage requirements. Core storage is reserved for a particular dimensional array only during the time the corresponding data are needed in the calculation, afterwards the array is released for other data.

6. **Typical Running Time:** Highly problem dependent, running time is affected by the parameters like the number of energy groups, number of dimensions (1, 2, 3), number of spatial intervals and PN approximation order used in the discrete ordinates transport calculations. The most complex case studied (VENUS-3 benchmark analysis [4] based on TORT 3D calculation using P-3/S-8 and 51/52/22 X/Y/Z intervals) took 2h40' on a PC Pentium.

7. **Unusual Features of the Program:** Although the sensitivities are calculated from the flux moment files, much smaller in size than the corresponding angular flux files, these files can still be voluminous for large 3D problems (see example in Section 11).
To simplify input preparation in 2D and in particular in 3D calculations the geometry description is read directly from the files produced by the discrete ordinates codes (see Section 8).
Modular structure of the code permits easy restart and supplementary calculations.

8. **Related and Auxiliary Programs:**

SUSD3D is loosely based on the SUSD code [6].

SUSD3D is coupled to several discrete-ordinates codes via binary interface files. For 1D analysis angular flux files from ANISN or flux moment files from ONEDANT can be used, for 2D analysis angular flux files from DOT-III or flux moment files produced by DORT or TWODANT, and for 3D analysis flux moment files produced by the TORT or THREEDANT codes. In some of these codes minor modifications are required. Variable dimensions used in the TORT-DORT system are supported. In 3D analysis the geometry and material composition is taken directly from the TORT produced VARSCL binary file, reducing in this way the user's input to SUSD3D.

Multigroup cross-section sets are read in the GENDF format of the NJOY/GROUPR [10] code system, and the covariance data are expected in the COVFIL format of NJOY/ERRORR or the COVERX format of PUFF-2.
The ZZ-VITAMIN-J/COVA [11] cross section covariance matrix library can be used as an alternative to the NJOY code system. The package includes the ANGELO code to produce the covariance data in the required energy structure in the COVFIL format.

The following modules are included in the package:

ERRORR34: an extension of the ERRORR module of the NJOY code system for the File-34 processing. It is used to prepare multigroup SAD cross sections covariance matrices.

GROUPSR: An additional code module for the NJOY code system to prepare partial cross sections for SAD sensitivity analysis. Updated version of the same code from SUSD, extended to the ENDF-6 format.

SEADR: An additional code module for the NJOY code system to prepare group covariance matrices for SAD/SED uncertainty analysis. As above.

9. **<u>Status</u>:** The code was successfully tested on sensitivity and uncertainty analyses for the PWR pressure vessel surveillance (using flux files from TWODANT), and analyses of the following benchmark experiments: ASPIS-Iron (ANISN and TWODANT), VENUS-3 (TORT), FNG Bulk Shield and FNG Streaming (both using DORT files). The final documentation is in preparation and the package will be available from the OECD/NEA Data Bank and from RSICC.

10. **<u>References</u>:**

1. I. Kodeli, *Progress on Computational Tools for 3D Sensitivity and Uncertainty Analysis*, Proc. OECD-NEA Seminar on 3D Deterministic Radiation Transport Computer Programs Features, Applications and Perspectives, Paris, 2-3 Dec. 1996.
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3. I. Kodeli, *Cross-Section Data Uncertainty and How Such Information is Used in Fusion Analysis*, Proc. Reg. Meeting on Nuclear Energy in Central Europe, Portorož, Slovenia (1999)

Background information and related codes:

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5. I. Kodeli, L. Petrizzi, P. Batistoni, *Transport, Sensitivity and Uncertainty Analysis of FNG 14 MeV Neutron Bulk Shield Experiment*, ICRS 9 conference, Tsukuba, Ibaraki, Japan (October 17-22, 1999)
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7. W. A. Rhoades, R. L. Childs, *TORT-DORT: Two- and Three-Dimensional Discrete Ordinates Transport*, Version 2.7.3, RSIC-CCC, ORNL RSIC, Oak Ridge, TN (1993)
8. R. E. Alcouffe et al., *DANTSYS 3.0 - A Diffusion-Accelerated, Neutral-Particle Transport Code System*, LA-12969-M, LANL (1995)
9. W. W. Engle, *A User's Manual for ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, Union Carbide Corporation (1967)

10. R. E. MacFarlane, D. W. Muir, *The NJOY Nuclear Data Processing System*, Manual LA-12740-M (1994).

11. I. Kodeli, E. Sartori, *ZZ-VITAMIN-J/COVA - Covariance Data Library*, OECD/NEA-DB, NEA 1264/03 package (1990).

11. **Hardware Requirements:** Core requirements depend on problem complexity. Up to eight tape units are used in addition to the standard input and output devices. The size of the flux moment files, produced by the TORT code for the above mentioned VENUS-3 benchmark analysis was 234 MB (two files required). For comparison, using the angular flux approach the corresponding file size would be 1407 MB.

12. **Programming Language(s):** FORTRAN-77.

13. **Operating System:** SUSD3D has run under MS-DOS on the personal computer using Lahey FORTRAN, Version 5.1; on DEC-VAX using VMS FORTRAN V6.1-386; and on HP/UNIX system.

14. **Other Programming or Operating Information or Restrictions:** None

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16. **Material Available:**

Reports [1] to [3] listed under Reference section and input manual (in preparation),
Fortran sources for SUSD3D, ERRORR34, GROUPSR and SEADR,
Command procedures,
Sample case input and output data

17. **Category:** D, O

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18. **Sponsor:** Institute Jožef Stefan; development was supported by European Fusion File (EFF) project of the European Community.