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Windows Interface Environment XSUN-2013 for OECD/NEA Transport and Sensitivity-Uncertainty Computer Codes TRANSX-2, PARTISN and SUSD3D

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ABSTRACT

A Windows interface XSUN-2013 facilitating the deterministic radiation transport and cross-section sensitivity-uncertainty calculation was developed. The package was developed to help users in the preparation of input cards, rapid modification and execution of the complete chain of codes including TRANSX, PARTISN and SUSD3D. It allows a user-friendly viewing of results obtained from PARTISN and SUSD3D programs. XSUN can produce 2D color schemes of PARTISN geometries (e.g. x-y, r-θ, ...) and different 3D plots (e.g. neutron flux distributions). The development of the tool was sponsored by the OECD/NEA and the package is available from the OECD/NEA Data Bank and RSICC since the beginning of 2014. Training courses are planned at NEA. An updated version is under final testing and will be released later this year.

1 INTRODUCTION

To respond to the needs of the users of the particle transport codes distributed by the NEA Data Bank a project of the development of a modern Windows interface environment was started two years ago sponsored by the NEA. Several of these high quality deterministic neutron transport codes, such as ANISN [1], DORT-TORT [2], DANTSYS [3], PARTISN [4] etc. were indeed developed in the 60-ies and 70-ies which use the computational standards of these times. Today these tools are less and less used, on one side due to the progress achieved in the Monte Carlo codes, and on the other due to the relatively archaic input formats used by these transport codes. However, the deterministic codes are still attractive for the use in many possible applications, be it for the sensitivity and uncertainty analyses, deep penetration problems and validation of Monte Carlo calculations. The motivation for this work was to facilitate the use of deterministic transport codes within a modern environment and thus bring these tools to the nowadays users.

2 COMPUTER CODE SYSTEM DESCRIPTION

The XSUN-2013 code package distributed through OECD/NEA Data Bank (Figure 1) and RSICC represents the first version of such user – computer interface for deterministic codes. The package is based on the Xbase++ (R) Compiler 1.90.331 and Alaska 32-Bit Linker [5], for the pre- and post-processing of the input and output data. It supports for now a limited, but complete and self-consistent set of deterministic codes with the following utility functions (see Figure 2):

- nuclear cross-section preparation (TRANSX-2-15 [6] code),
- transport of neutral particles for criticality and shielding calculations (code PARTISN [4]),
- nuclear data sensitivity and uncertainty calculations (code SUSD3D [8]).

All the above codes are available from the OECD/NEA Data Bank and RSICC. These codes were usually considered to be difficult to use. Objective of this work was to make the input and output handling for these codes as user friendly as possible, passing information among the codes internally.

2.1 TRANSX-2.15 [6]

TRANSX is a computer code that reads nuclear data from a library in MATXS format and produces transport tables compatible with many discrete-ordinates (S_N) and diffusion codes. MATXS format libraries are prepared using the NJOY-99 [7] code (or more recent versions). Tables can be produced for neutron, photon, charged-particle, or coupled transport. Options include adjoint tables, mixtures, homogeneous or heterogeneous self-shielding, group collapse, homogenization, thermal upscatter, prompt or steady-state fission, transport corrections, elastic removal corrections, and flexible response function edits.

TRANSX reads through the materials in a MATXS library and accumulates the cross sections into a transport table using the user's mix instructions. At the same time, response function edit cross sections are accumulated using the user's edit instructions. They can thus be any linear combination of the cross sections available in the library. When the table is complete, it is written out in the desired format. Output options include DTF-style card images, FIDO, ISOTXS, and the binary group-ordered GOXS format.

TRANSX is written in FORTRAN-77 and runs under DOS, LINUX and UNIX operating systems.

2.2 PARTISN [4]

PARTISN (PARallel, TIme-Dependent SN) is a relatively recent S_N transport code for shielding and criticality calculations and the evolutionary successor to CCC-547/DANTSYS. The code is a modular computer program package designed to solve the time-independent or dependent multigroup discrete ordinates form of the Boltzmann transport equation in several different geometries. The modular construction of the package separates the input processing, the transport equation solving, and the post processing (or edit) functions into distinct code modules: the Input Module, the Solver Module, and the Edit Module, respectively. The Input and Edit Modules in PARTISN are very similar to those in DANTSYS. However, unlike DANTSYS, the Solver Module in PARTISN contains one, two, and three-dimensional solvers in a single module. In addition to the diamond-differencing method, the Solver Module also has Adaptive Weighted Diamond-Differencing, Linear Discontinuous, and Exponential Discontinuous spatial differencing methods. The spatial mesh may consist of either a standard orthogonal mesh or a block adaptive orthogonal mesh. The Solver Module may be run in parallel for two and three dimensional problems. One can run 1-D problems in parallel using Energy Domain Decomposition.

Both the static (fixed source or eigenvalue) and time-dependent forms of the transport equation are solved in forward or adjoint mode. In addition, PARTISN has a probabilistic mode for Probability of Initiation (static) and Probability of Survival (dynamic) calculations. Vacuum, reflective, periodic, white, or inhomogeneous boundary conditions are solved. General anisotropic scattering and inhomogeneous sources are permitted. PARTISN solves

the transport equation on orthogonal (single level or block-structured AMR) grids in 1-dimensional (slab, two-angle slab, cylindrical, or spherical), 2-dimensional (X-Y, R-Z, or R-T) and 3-dimensional (X-Y-Z or R-Z-T) geometries.

PARTISN is written in FORTRAN-95 and runs under Linux, DOS Windows, and UNIX operating systems.

2.3 SUSD3D [8]

XSUN-2013 includes the latest improved and extended version of the SUSD3D multi-dimensional nuclear cross-section sensitivity and uncertainty code, based on the first-order generalised perturbation theory. The code calculates the sensitivity coefficients and standard deviation in the calculated detector responses or design parameters of interest due to the input cross sections and their uncertainties. Complex 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.

Either relative $\left(\frac{\sigma}{R}\frac{dR}{d\sigma}\right)$ or absolute $\left(\frac{1}{R}\frac{dR}{d\sigma}\right)$ sensitivities can be calculated, the latter being used for the SEMOVE/GANDR [9] program.

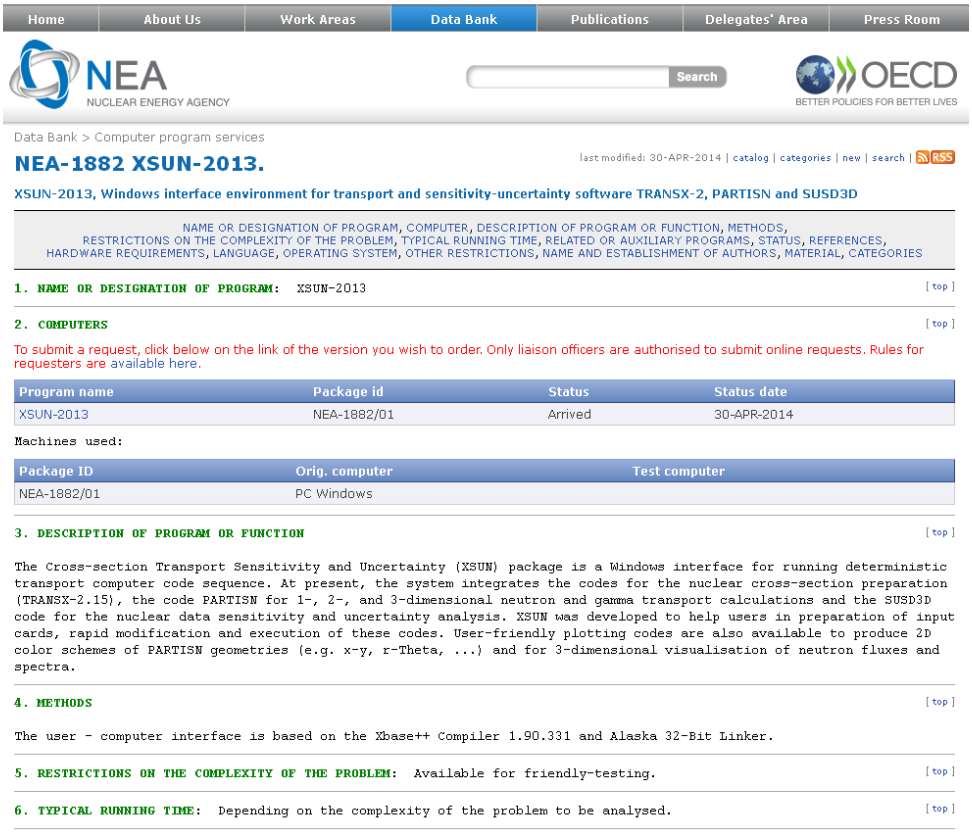
The particle transport calculations are done externally using the existing codes, which guarantees great flexibility and allows the use of the most up-to-date transport codes. At present SUSD3D can use the neutron/gamma flux moment files produced by the DORT, TORT [2], ONEDANT, TWODANT, THREEDANT [3] and PARTISN discrete ordinates codes or the angular flux files from the ANISN [1] and DOT-III codes. Updates for the other codes such as DRAGON and ATTILA are under preparation in the scope of F4E project and as part of a PhD thesis.

The sensitivity profiles are folded with the cross section covariance matrices to determine the variance in an integral response of interest. Uncertainties due to the fission spectra uncertainties can be calculated either using the classical or the constrained sensitivity method [7, 8], useful particularly in case the fission spectra covariance matrices do not comply exactly with the ENDF-6 Format Manual rules.

Development of SUSD3D started in early 1990-ies in the scope of the French pressure vessel surveillance programme and the EC fusion project. The code runs under DOS Windows and LINUX using FORTRAN-95 compiler.

Several innovative mathematical methods were developed in the scope of the SUSD3D project, such as:

- Constrained sensitivity method to calculate the sensitivity to the secondary energy distributions, such as fission spectra sensitivities [10],
- Sensitivity and uncertainty calculations of the effective delayed neutron fraction (β_{eff}) [11].



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NEA-1882 XSUN-2013.

XSUN-2013, Windows interface environment for transport and sensitivity-uncertainty software TRANSX-2, PARTISN and SUSD3D

NAME OR DESIGNATION OF PROGRAM, COMPUTER, DESCRIPTION OF PROGRAM OR FUNCTION, METHODS, RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM, TYPICAL RUNNING TIME, RELATED OR AUXILIARY PROGRAMS, STATUS, REFERENCES, HARDWARE REQUIREMENTS, LANGUAGE, OPERATING SYSTEM, OTHER RESTRICTIONS, NAME AND ESTABLISHMENT OF AUTHORS, MATERIAL, CATEGORIES

1. NAME OR DESIGNATION OF PROGRAM: XSUN-2013 [top]

2. COMPUTERS [top]

To submit a request, click below on the link of the version you wish to order. Only liaison officers are authorised to submit online requests. Rules for requesters are available here.

Program name	Package id	Status	Status date
XSUN-2013	NEA-1882/01	Arrived	30-APR-2014

Machines used:

Package ID	Orig. computer	Test computer
NEA-1882/01	PC Windows	

3. DESCRIPTION OF PROGRAM OR FUNCTION [top]

The Cross-section Transport Sensitivity and Uncertainty (XSUN) package is a Windows interface for running deterministic transport computer code sequence. At present, the system integrates the codes for the nuclear cross-section preparation (TRANSX-2.15), the code PARTISN for 1-, 2-, and 3-dimensional neutron and gamma transport calculations and the SUSD3D code for the nuclear data sensitivity and uncertainty analysis. XSUN was developed to help users in preparation of input cards, rapid modification and execution of these codes. User-friendly plotting codes are also available to produce 2D color schemes of PARTISN geometries (e.g. x-y, r-Theta, ...) and for 3-dimensional visualisation of neutron fluxes and spectra.

4. METHODS [top]

The user - computer interface is based on the Xbase++ Compiler 1.90.331 and Alaska 32-Bit Linker.

5. RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM: Available for friendly-testing. [top]

6. TYPICAL RUNNING TIME: Depending on the complexity of the problem to be analysed. [top]

Figure 1: XSUN-2013 computer code page at OECD/NEA Data Bank

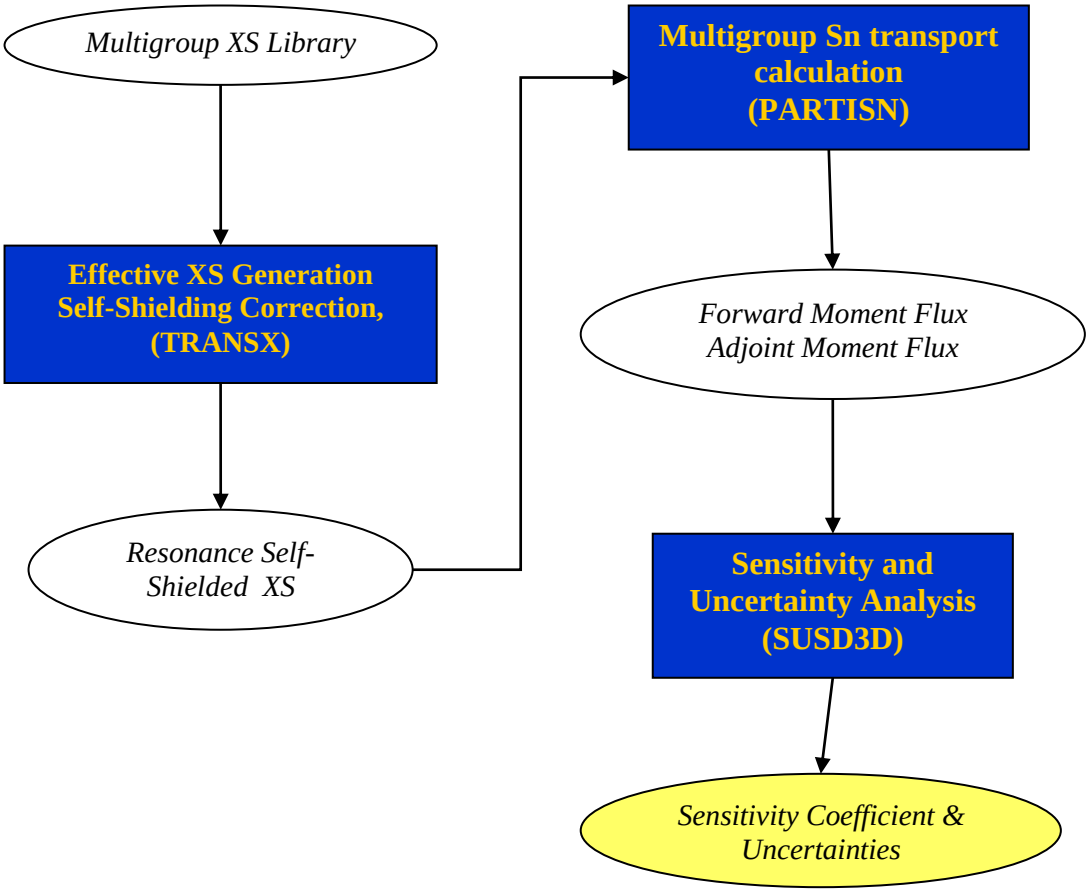

Figure 2: XSUN-2013 computer code system

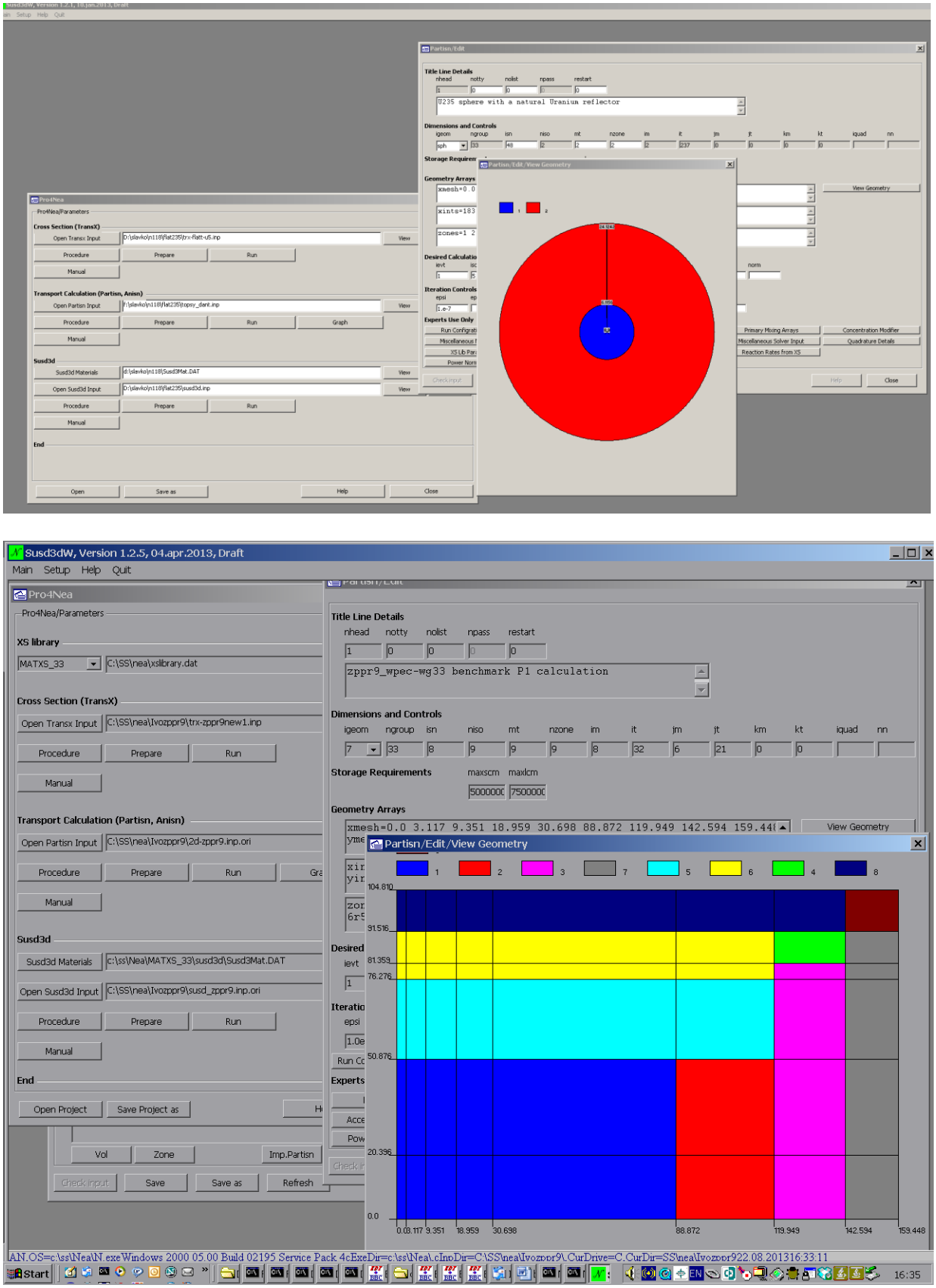

Figure 3: Screen captures of the PARTISN test case 1 and 2 running sequences

3 CONCLUSIONS

A modern computer code interface XSUN-2013 was developed for the preparation and execution of the deterministic neutron-gamma computer codes in a user friendly way adopted for today standards and users. At present, the system integrates the codes for the nuclear cross-section preparation (TRANSX-2.15), the code PARTISN for 1-, 2-, and 3-dimensional neutron and gamma transport calculations and the SUSD3D code for the nuclear data sensitivity and uncertainty analysis. User-friendly plotting codes are also available for the 3-dimensional visualisation of neutron fluxes, spectra and sensitivity profiles (Fig. 3). XSUN-2013 system is available through the OECD/NEA Data Bank and RSICC since early 2014. Several copies of the system were already distributed and the system was successfully used by students at the Jožef Stefan Institute. An updated and improved version is under testing and will be released later this year.

ACKNOWLEDGMENTS

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