Recent Development and Examples of Use of the Windows Interface Environment XSUN-2016 for Transport and Sensitivity-Uncertainty Analysis

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ABSTRACT

In 2013 the first version of the Windows interface XSUN-2013 facilitating the deterministic radiation transport and cross-section sensitivity-uncertainty (S/U) calculation was developed and submitted to OECD/NEA Data Bank Computer Code Collection and RSICC. The package allows the preparation of input cards, rapid modification and execution of the complete chain of codes including TRANSX, PARTISN and SUS3D in a user-friendly way. A new version of the code, XSUN-2016, including several major modifications and improvements will be released this year. Description and few examples of the use of XSUN-2016 are presented, including:

- S/U intercomparison exercise using the SNEAK-7A & -7B benchmark experiments from the IRPhE database. The performance of the XSUN-2016 code system was compared with the codes such as TSUNAMI, SERPENT and MCNP6.
- Transport, sensitivity and uncertainty analysis of the \( k_{\text{eff}} \) and \( \beta_{\text{eff}} \) parameters for the MYRRHA accelerator driven system (ADS).

1 INTRODUCTION

In order to facilitate the use of the deterministic particle transport codes, in decline as compared to the more and more widely used Monte Carlo codes, a project of the development of a modern Windows interface environment was started in 2012 initially sponsored by the NEA Data Bank. Several of the high quality deterministic neutron transport codes, such as ANISN [1], DORT-TORT [2], DANTSYS [3], PARTISN [4] date back to the 60-ies and 70-ies and have difficulties to meet the “comfort” expectations of nowadays users, therefore today less and less used. 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 XSUN COMPUTER CODE SYSTEM

The XSUN-2013 [5] code system was released in spring 2014 to OECD Nuclear Energy Agency Data Bank (Package-ID NEA-1882) and RSICC (Code Number CCC-825). The package can be obtained from the two data centers, by contacting the RSICC or NEA Data Bank Computer Program Services or one of the nominated establishments in your country. An updated version of the code system, XSUN-2016, will be released later this year.

The XSUN-2016 code package is a user – computer interface environment integrating several deterministic codes and organised in a way to make the input and output handling for these codes as user friendly as possible, passing information among the codes internally to assure input data preparation in a consistent way. The package is based on the Xbase++ (R) Compiler 1.90.331 and Alaska 32-Bit Linker [6], 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, all available from the OECD/NEA Data Bank and RSICC, with the following utility functions:

i) Multi-group nuclear cross-section preparation (TRANSX-2-15 [7] code): 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 [8] code (or more recent versions). Tables can be produced for neutron, photon, charged-particle, or coupled transport. Options include adjacent 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. The output self-shielded multigroup cross sections for the mixtures according to the user’s mix instructions can be written in DTF-style card images, FIDO, ISOTXS, or the binary group-ordered GOXS format.

2) Transport of neutral particles for criticality and shielding calculations (code PARTISN [4]): PARTISN (PARallel, TIme-Dependent SN) is a discrete ordinates (S_N) transport code for shielding and criticality calculations. 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. 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.
3) Nuclear data sensitivity and uncertainty calculations (code SUSD3D [9]): The development of SUSD3D started in early 1990-ies in the scope of the French pressure vessel surveillance programme and the EC fusion project. XSUN-2016 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 multi-group cross sections, (2) energy-dependent response functions, (3) secondary angular distribution (SAD) or secondary energy distribution (SED) uncertainties.

The particle transport calculations are done externally using the existing codes (such as PARTISN in this case), and the information on the direct and adjoint fluxes is passed to SUSD3D via the neutron/gamma flux moment files calculated by PARTISN. This guarantees great flexibility in the choice of the transport solver and allows the use of the most up-to-date transport codes. For example, the present version of SUSD3D can use. In addition to PARTISN, 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 ATTLA 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. Several innovative mathematical methods were developed in the scope of the SUSD3D project, which were later introduced also in other codes such as TSUNAMI, SERPENT, MCNP such as:

- Demonstration of the equivalence of the Constrained sensitivity method and covariance matrix fix-up in the calculation of the sensitivity to the secondary energy distributions, such as fission spectra sensitivities [10]. The constrained sensitivity method is useful particularly in cases where the fission spectra covariance matrices do not comply exactly with the ENDF-6 Format Manual rules;

- Sensitivity and uncertainty calculations of the effective delayed neutron fraction ($\beta_{\text{eff}}$) [11].

4) Several nuclear cross-section and covariance matrix libraries are available with the XSUN-2016 package. The following multi-group cross-section libraries are to be utilised in TRANSX/PARTISN code suite:

- Nuclear cross section data library in the ECCO 33-neutron energy group structure, in MATXS format. The library includes data for 109 isotopes at different temperatures (300 K, 550 K, 600 K, 650 K, 700 K, 800 K) and for different self-shielding factors. The data were produced using the NJOY-99 code and are based mostly on the ENDF/B-VII.1 nuclear data evaluation (with some date from the -VII.0 release).

- FENDL-3.1 211 neutron group cross sections can be extracted from IAEA site https://www-nds.iaea.org/fendl3/ for fusion application. The data were processed at the IAEA.

The above neutron cross sections are also available in the GROUPR format to be used in the code SUSD3D for the proper normalisation of the sensitivity profiles.
5) The following multi-group covariance matrix libraries are available with the XSUN-2016 package:
   - ENDF/B-VII.1 covariance matrices processed using the NJOY-99 code in the ECCO 33 energy groups
   - JENDL-4.0 covariances processed using the NJOY-99 code in the ECCO 33 energy groups
   - SCALE-6.0m covariances [12] processed using the ANGELO code (ECCO 33 energy groups)
   - Detector response functions from the IRDFF evaluation (33 group structure).

2.1 Modifications since the official XSUN-2013 release

XSUN is an active project and is continuously being developed and updated at JSI in spite of no specific funding received after the initial financing by OECD/NEA. Since the beginning of the project in 2012 altogether 149 versions of the XSUN package were prepared. Some of the recently implemented features since the XSUN-2013 version include:

TRANSX:
   - For very large problems (mixs>1000)
   - The default ENDF/B-VII.1 cross sections library was updated with new materials, several temperatures and self-shielding tables
   - Other libraries such as FENDL-3 (211 energy groups) were tested

PARTISN:
   - Corrections for input preparation of 3-dimensional problems (space mesh and zones)
   - Multilines in case of lines exceeding 80 characters (e.g. specification of x-y-z mesh coordinates, zone assignment)
   - External source specifications allowed

SUSD3D input preparation (many modifications, corrections, updates):
   - Preparation of the Overlays 2 and 3 specifying the list of materials and reactions for which the sensitivities and uncertainties are calculated was completely re-organised and automatized using internally the TRANSX and PARTISN input decks. The material and reaction list is constructed according to the selected cross section and covariance files selected and requires little user's intervention. User can select among several temperatures available in the cross section library;
   - Energy dependent self-shielding factors are taken directly from the TRANSX output (ongoing modifications)
   - Consistency checks between SUSD3D/TRANSX and SUSD3D/PARTISN inputs
   - Major corrections and updates in the space mesh conversion from the PARTISN input, in particular for 3D geometries
   - Multilines in case of lines exceeding 80 characters (e.g. specification of x-y-z mesh coordinates)
- For the visualisation of the sensitivity profiles, a link to the user-friendly “Sensitivities Plots” [13] utility was introduced.

Several other modifications and improvements such as Project test case save/open features, File history cleaning button, etc. were introduced.

2.2 Modifications in the SUSD3D code

Several improvements were introduced also in the main SUSD3D code used for the S/U calculations, in particular:

- Treatment of self-shielding factors ($\sigma_0$) for the cross sections used in SUSD3D for the normalisation of the sensitivities: one fixed energy independent $\sigma_0$ factor selected from the values in the multi-group cross-section file was used in the previous version. The new code now allows the interpolation among the $\sigma_0$ tables in the file. Energy dependent $\sigma_0$ values, as calculated in the TRANSX code, can be used allowing the full consistency between the cross section used in the transport calculation (PARTISN) and for the SUSD3D sensitivity calculations.

- A bug in the code for the 3D PARTISN calculations was corrected

- The uncertainty in the secondary angular distributions (SAD) can be calculated using the covariance matrices provided in the MT=251 file format for the $P_1$ Legendre terms.

- Several minor modifications and improvements

The TRANSX code was also updated to increase the memory size (for large problems) and allow the self-shielding print on a separate file to be used subsequently in XSUN-2016 for the SUSD3D input preparation. An error was corrected to make the code compatible with modern (and less permissive) compilers.

3 USE AND VALIDATION

Few examples of the recent use of the XSUN-2016 system include e.g.:

- S/U inter-comparison exercise using the SNEAK-7A & -7B benchmark experiments [14, 15] from the IRPhE database. The performance of the XSUN-2016 code system was compared with the codes such as TSUNAMI, SERPENT and MCNP6.

- Transport, sensitivity and uncertainty analysis of the $k_{eff}$ and $\beta_{eff}$ parameters for the MYRRHA accelerator driven system (ADS) [16, 17].

3.1 Sensitivity code inter-comparison using SNEAK-7 benchmarks

A sensitivity benchmark exercise was organized within the scope of the Uncertainty Analysis in Modeling (UAM) project [18, 19] of the OECD/Nuclear Energy Agency (NEA) to develop and compare the available methods for the sensitivity and uncertainty computations of the effective multiplication factor ($k_{eff}$) and the effective delayed neutron fraction ($\beta_{eff}$). Several solutions of the $k_{eff}$ S/U results were received using different codes (see Fig. 1), both deterministic (SUSD3D, SNATCH) and Monte Carlo (TSUNAMI-3D, XSUSA, SERPENT2, MCNP6). The sensitivity and uncertainty codes were applied to the SNEAK-7A and -7B [20] fast neutron benchmark experiments from the IRPhE database. The sensitivity coefficients of $\beta_{eff}$ with respect to the basic nuclear data were calculated by deriving the Bretscher's k-ratio
formula as initially proposed in 2010 following the interest expressed in the scope of the UAM project. For the $\beta_{\text{eff}}$ S/U calculations the solutions obtained using the codes SUSD3D, SERPENT and XSUSA were compared (Fig. 2).

AS can be seen on Figs. 1 and 2, good general agreement between the sensitivities, both for integral values and sensitivity profiles, was observed.

![Graphs showing sensitivity to U238 elastic and inelastic cross sections calculated by SUSD3D, SERPENT, TSUNAMI3D, MCNP6, and SNATCH codes.]

Figure 1: Example of most discrepant sensitivities of $k_{\text{eff}}$ to $^{238}\text{U}$ elastic and inelastic cross sections calculated by SUSD3D, SERPENT, TSUNAMI3D, MCNP6 and SNATCH codes.
3.2 MYRRHA ADS reactor S/U analysis

MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications) [16] is being designed at SCK•CEN, Mol, Belgium conceived to operate both in sub-critical (Accelerator Driven System-ADS) and in critical mode. In the scope of the CHANDA project of the EC 7th Framework Programme a sensitivity and uncertainty analysis of the neutron multiplication factor $k_{eff}$ and the effective delayed neutron fraction $\beta_{eff}$ were performed to identify the most important nuclear data for neutron-induced reactions for criticality calculations of the latest MYRRHA designs. The sensitivity profiles were calculated using different, both stochastic and deterministic, codes (i.e. SCALE/TSUNAMI, MCNP and XSUN/SUSD3D). MCNP and TSUNAMI calculations were performed using a detailed 3D geometry model. A simplified 2D r-z geometrical model was prepared for SUSD3D (and TSUNAMI) based on the detailed MCNP model of MYRRHA. The problem was still relatively large, with the dimensions of 5 m (r-direction) and 8.5 m (z-direction), 24 material mixtures with 1257 materials at different temperatures from 300 K to 800 K. 33-group cross sections were used in PARTISN and SUSD3D calculations, pointwise data in MCNP and 238 energy group library in SCALE/TSUNAMI codes.

In spite of the differences in S/U methodologies, different cross section energy representations and cross section processing and treatment, the neutron-induced nuclear data sensitivity analysis resulted in differences of less than 4% between codes, with few exceptions ($^{239}$Pu fission, $^{238}$U elastic scattering and $^{56}$Fe capture reactions). Nuclear data covariance matrices of different libraries (SCALE-6, COMMARA-2 and JENDL-4.0m) were used to derive the uncertainty in $k_{eff}$ based on the calculated sensitivities. This study concluded that, depending on the covariance data used, the $k_{eff}$ and $\beta_{eff}$ uncertainties due to the uncertainty in nuclear data were about 0.5-1% and ~2.2%, respectively.
Figure 3. XSUN-2016 computational running segment with the view of the MYRRHA geometry modeling

Figure 4. Distribution of the thermal neutron flux in MYRRHA calculated using the PARTISN code (plotted by N. Soppera, MeshTal Viewer)
Figure 5. Distribution of the 1-2 keV neutron flux in MYRRHA calculated using the PARTISN code (plotted by N. Soppera, MeshTal Viewer)

Figure 6. Distribution of ~3 MeV neutron flux in MYRRHA calculated using the PARTISN code (plotted by N. Soppera, MeshTal Viewer)
Figure 7. Sensitivity of $k_{\text{eff}}$ calculated using the SUSD3D and TSUNAMI codes for the MYRRHA reactor.

Figure 8. Sensitivity of $\beta_{\text{eff}}$ to the total neutron yield of $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu and $^{241}$Pu calculated using the SUSD3D code for the MYRRHA reactor.

4 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, XSUN-2016, is under testing and will be released later this year.

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REFERENCES


ZZ-Scale6/COVA-44G, OECD/NEA PACKAGE-ID: USCD-1236/02 (May 2009), USCD-1236/03 (May 2012)


