CM on Data Processing Codes

Questionnaire on the data processing codes used in different laboratories
Feedback provided by

IAEA-NDS A. Trkov, International Atomic Energy Agency, Vienna, Austria
BNL-NNDC D. Brown, Brookhaven National Laboratory, National Nuclear Data Center
OECD/NEA Data Bank, Nuclear Data team
LLNL B. Beck, Lawrence Livermore National Laboratory
JAEA Ken-ichi Tada, Japan Atomic Energy Agency
CNDC Liu Ping, China Nuclear Data Centre
NRC KI V.Sinitsa, National Research Centre "Kurchatov Institute", Moscow, Russia
KAERI-NDC Do Heon Kim, Korea Atomic Energy Research Institute, Nuclear Data Center

- **What is the end purpose of your data processing activities?**

IAEA The main purpose is data verification and validation and pre-processing for graphical display. Additional activity is the preparation of special-purpose transport libraries, libraries for neutron dosimetry, activation (including charged particles) and Standards.

NNDC The NNDC has several purposes for data processing, but chief among these is data testing of the ENDF/B nuclear data library. ENDF library users expect ENDF data to be physically correct and to process cleanly through whatever processing system they use in house. This means the NNDC aims to demonstrate that all ENDF files in the current ENDF library can be processed through all user codes in the intended manner. Naturally we are far from this goal. All of our processing is done within the context of the NNDC continuous integration system called ADVANCE.

OECD/NEA Data Bank has developed NDEC system for nuclear data verification to enhance Nuclear Data Services and to serve the production of JEFF libraries. The NDEC is a systematized workflow for handling and diagnosing the quality of nuclear data under the different steps involved in the production of nuclear data libraries. These steps are the verification, processing, experimental differential validation and experimental integral benchmarking of evaluated nuclear data files. By the NDEC system, special attention will be paid to the identification of bugs in files, and the development of file and processing standard formats (ACE, APMX, MATXS, ...).

LLNL We serve LLNL nuclear data users. They require viewing, manipulation (e.g, Kiwi) and processing (e.g., grouping data for deterministic and Monte Carlo transport) of the nuclear data as well as a suite of functions that check the physics, where possible, of the data.

JAEA We use the data processing code to make the cross section library for our nuclear calculation code, e.g., SRAC and SLAROM-UF for the deterministic code and MVP and PHITS for the continuous energy Monte Carlo code. The final purpose of our data processing activities are publication of these cross section library to the calculation code users.

CNDC Data testing of CENDL nuclear data libraries

Preparation of application libraries from evaluated data files

NRC KI The purpose of our processing activity is:

creation computation tool for preparation and verification pointwise, multigroup and subgroup (probabilistic) data from evaluated data files and integral experiments for nuclear engineering: reactor physics, radiation shielding, neutron dosimetry, fuel handling and storage, criticality safety;

preparation and validation working data libraries for deterministic and Monte Carlo application codes.

KAERI The main purpose is to generate several kinds of cross section libraries for radiation transport/depletion calculations and disseminate them to many researchers in domestic and foreign institutions, while fulfilling the nuclear data needs for research and development activities on the advanced reactors. We also perform nuclear data processing to verify and validate our new evaluated data.

- **Which application code uses your processed data (is it open source, available on request or classified)?**

IAEA Whenever possible, open source codes are used; these include codes that are available through various projects (RR_UNC, GRUPINT), ENDVER for data display and comparison with experimental data. The primary tool for the validation of transport libraries is the MCNP Monte Carlo code.

NNDC Our processed data is used in benchmark simulations performed with MCNP and COG. We are considering exploring OpenMC and SCALE.

OECD/NEA Data Bank Validation of processed data with MCNP (with NJOY2012) and SCALE (AMPX). Application in different Benchmarks (ICSBEP – criticality and spectral indexes, SINBAD, IRPhE, …).

LLNL We have many application codes. None, to my knowledge, is open source.

JAEA We use the NJOY99 and the PREPRO code. Now, we also use the NJOY2012 code for a test processing. However, we use the NJOY99 and the PREPRO code to make the new cross section library for publication.

CNDC Our processed data is used in benchmark simulations performed with MCNP

Our processed data is also used in benchmark simulations performed with some Sn code, such as SCALE4.3

NRC KI Our processed data was supplied to SAPFIR, MCU (NRC "Kurchatov Institute"), RADUGA, REACTOR (Keldysh Institute of Applied Mathematics, KIAM), CONSYST (A.I. Leipunski Institute of Physics and Power Engineering, IPPE), C4R/C4P/SIMMER (Karlsruhe Institute of Technology,KIT). None are open source.

KAERI We usually use open source application codes such as MCNP/MCNPX, DANTSYS, DOORS, SCALE, SUSD3D, etc. to validate our processed cross section libraries. We also have some application codes (e.g., McCARD and MUST) compatible with NJOY/TRANSX-processed libraries and other application codes (e.g., DeCART, nTRACER, LIBERTE, and KARMA) with their own library formats. These Korean made codes except for McCARD may not be open to the public.

- **What is the processed data format?**

IAEA Dosimetry and activation libraries used in conjunction with codes like RR_UNC and GRUPINT use the ENDF-like format for cross sections with histogram interpolation. The MCNP code uses the ACE format. Special purpose libraries (e.g. FENDL-3, ADS) are also generated in the MATXS format, but with limited QA.

NNDC MCNP uses the ACE format and COG can use ACE or raw ENDF.

OECD/NEA Data Bank: The aim is providing enlarged and enhanced nuclear data services to OECD/NEA DB member countries in the framework of processing, verification and benchmarking of evaluated nuclear data: ACE format for MCNP, AMPX format for SCALE,… and others.

LLNL We are planning to use GND as it supports storing both evaluated and processed data. Fudge generates processed data in the GND format. However, we plan to support the conversion of GND data to other formats. For example, we already have a GND to ACE converter that is nearly complete for neutrons. Since the interface to Fudge is Python, it is relatively simple to convert GND processed data to other process formats. (Note, the first sentence says 'planning' because LLNL currently uses other formats that are old and that we

are deprecating. In my opinion, these deprecated formats are of no use to others).

JAEA Our deterministic nuclear calculation code uses the original data format. The energy group structure of the SRAC code is 107 groups and that of the SLAROM-UF code is three different energy group structures, i.e., 70, 175 and 900 groups.

For the continuous energy Monte Carlo code, the MVP code uses our original data format and the PHITS code uses the ACE format.

CNDC MCNP uses the ACE format,

WIMS-D/WIMS-D+ format

SCALE4 uses the AMPX format

NRC KI Domestic formats: BNAB, TEMBR;

Other widely used formats: NJOY internal formats – PENDF, GENDF; ENDF (for restricted set of data types); ACE (at present time – not for all materials, due to restrictions in processing MF6 file).

KAERI We generate the ACE-format library for MCNP/MCNPX and McCARD codes, the MATXS-format library for DANTSYS and DOORS code systems, and the WIMS-format library for WIMS-D code. We use the COVFIL-format covariance data library for SUSD3D code. The DeCARD, nTRACER, LIBERTE, and KARMA codes use their own library formats suitable for PWR core analyses.

- **What are the characteristics of the group structure if preparing data for deterministic codes?**

IAEA Fine group for dosimetry and activation libraries (640-group SAND-II, 725-group extended SAND-II spanning the range from 1.E-5 eV to 60 MeV; continuous energy for ACE libraries, different group structures for FENDL and ADS libraries)

NNDC n/a

OECD/NEA Data Bank Continuous energy (CE) for ACE and AMPX libraries; Multi-group (MG) for SCALE.

LLNL We are planning to be as flexible as possible. Any group energy boundaries and flux can be used. When Fudge is released with processing, anyone can use

it to create their own processed data in the GND format. All they will need is to write a converter to convert GND into their processed format.

JAEA For the SRAC code, the fast group is divided by equal lethargy width. Though the thermal group is divided finer than equal lethargy width, the detail concept of the thermal energy group structure is unknown.

The new version of the SRAC code will adopt 200 energy groups structure. The energy group structure is similar to 172 groups XMAS energy group structure. To improve the prediction accuracy of the shielding calculation, the cross section of Iron is treated finer.

For the SLAROM-UF code, the characteristics of each energy group structure are different. 70 energy groups structure is divided by equal lethargy width. 175 energy groups structure adopts the VITAMIN energy group structure and adds 12.84MeV. 900 energy groups structure is divided by equal lethargy width. To consider the average lethargy increase by the elastic scattering of 238U, the lethargy width is modified at 50 keV. When the neutron energy is less than 50 keV, the lethargy width is 0.050-0.120. When the neutron energy is larger than 50 keV, the lethargy width is 0.008. To conform 175 energy groups structure, some energy groups are modified.

CNDC Continuous energy point for ACE libraries

We are designing a flexible group structure. The basic method is to generate the main library with fine group structure, and working library with broader group structure. The interface code from main library to working library is under development.

NRC KI Any group energy boundaries, standard set of parametric and tabulated weight functions.

KAERI The shielding library, KASHIL has been tested with many different energy group structures, i.e., VITAMIN-B6 (199-g N & 42-g G), VITAMIN-J (175-g N & 42-g G), LANL (80-g N & 24-g G), BUGLE (47-g N & 20-g G), SCALE (44-g N & 18-g G), and LANL (30-g N & 12-g G). The fast reactor library, KAFAX uses LANL (80-g N & 24-g G) and KAFAX (150-g N & 12-g G) energy group structures. The KAFAX neutron group structure consists of one-eighth lethargy widths in almost all energy ranges, except between 1 and 10 keV in which one-sixteenth lethargy widths are used. The master library for PWR core analysis codes use HELIOS neutron group structure of 190-group.

- **What is the status of your data processing code (e.g.: open source, available on request, classified, under development, etc.)?**

IAEA PREPRO and ENDVER are open source, maintained by the IAEA; NJOY is a processing system obtained from LANL and used under license.

NNDC We currently use Fudge (LLNL), NJOY (LANL), PREPRO (IAEA), the NNDC checking codes (not really processing…) in ADVANCE. We have a goal to implement AMPX (ORNL) in ADVANCE. D. Brown is also a co-developer of Fudge, focusing on the resonance processing and tools for evaluation checking and repair. Of these codes, only Fudge is open source and the latest release was under the GNU Public License. Future Fudge releases will be under the BSD license so that Fudge may be incorporated into proprietary code systems.

OECD/NEA Data Bank: For checking and verification, PREPRO and ENDVER are open source. For processing NJOY2012 from LANL and SCALE/AMPX used under license. For integral comparison and visualization, JANIS tool developed. For Benchmarking purposes DICE system is used. JANIS and DICE are developed by NEA.

LLNL Our processing code will be a part of Fudge and Fudge is open source and not export controlled. We have already released several versions of Fudge without processing under the GNU Public License. Our next release as well as other future releases will be under the BSD license. Soon we will include our processing codes with Fudge. Our Fudge-based deterministic processing codes were recently developed and we are testing them against NJOY (LANL) and AMPX (ORNL).

JAEA In the previous century, we developed own nuclear data processing code. However, we stopped the development of the processing code and we currently use the NJOY99 and the PREPRO code.

CNDC NJOY99: Obtained from LANL and used under license

PREPRO: Obtained from IAEA

Ruler: we developed own nuclear data processing code

NRC KI It depends on the set of functional modules included to the package.

The existing GRUCON-D (“demo”) set includes only modules needed for resonance structure description and ACE file preparation (presently, with restrictions); it can be requested and is freely available for non-commercial use. T

The GRUCON-B (“basic”) will include total set of updated modules from previous version of GRUCON (some of modules were developed for ENDF/B-V data library and became obsolete). Now it is under development, the future status is not yet defined.

KAERI We are using NJOY99/NJOY2012 (LANL), ERRORJ (JAEA), AMPX/PUFF-IV (ORNL), and PREPRO (IAEA) codes. We do not have our own nuclear data processing code, but some auxiliary tools have been developed to ease the NJOY processing and generate the unique master library for PWR core analysis codes.

- **If enhancement of the open-source data processing capabilities is undertaken through the IAEA, are you willing to contribute your software?**

IAEA We are considering engagement in an activity to develop a module to generate multi-band parameters (equivalent to probability tables) in the resonance range. We are also working on the implementation of GRUCON, which will be freely available for non-commercial purposes.

NNDC We also hope Fudge (already an open source code) can be part of this effort. We will likely implement whatever capabilities developed through the IAEA in our ADVANCE code, especially if these capabilities are open source.

OECD/NEA Data Bank may contribute for verification and benchmarking of new enhancements using NDEC system.

LLNL The repo for Fudge will be owned by LLNL so that we can verify what is in Fudge. That said, our code is released for all to use and we welcome any comments and contributions. All contributions will need to be vetted by LLNL before they can be added to Fudge.

JAEA For JAEA, it is absolutely difficult to contribute the development of the open source code. We may contribute as the benchmark, e.g., comparing the cross section data library which is made by JAEA and open source code.

CNDC It is relatively difficult to contribute our own nuclear data processing code. We may contribute the comparison of the cross section data library generated with NJOY code.

NRC KI It is not forbidded to add to the GRUCON package a new module as “open source”. We are ready to cooperate in development of such modules.

KAERI Maybe we cannot directly contribute our efforts to enhancement of the open-source nuclear data processing code. However we are willing to participate in validation study of the code.

- **Which in your opinion are the data processing modules of highest priority that are not available as open-source software?**

IAEA Processing of cross sections in the unresolved resonance range, preparation of scattering matrices for deterministic codes.

NNDC - Probability table methods such as PURR (NJOY) or PURM (AMPX). We aim to implement this in Fudge in the near future. Also, WPEC-SG38 will result in major changes to the ENDF format. At least one open source code other than Fudge must be capable of handling data in this format so that we can do cross checking.

- Open-source implementation of LEAPR for thermal scattering data. We (as a community) rely exclusively on NJOY, so we should worry about cross checking.

OECD/NEA Data Bank will work to enlarge and enhance nuclear data services to member countries in the framework of processing, verification and benchmarking of evaluated nuclear data. Software based on open-source or under license will be used.

OECD/NEA-DB/CPS has served as repository to processing tools (e.g. NJOY, http://www.oecd-nea.org/dbprog/njoy-links.html), including links to official and un-official updates.

LLNL Currently, our processing is not included in a Fudge release. But this will change soon (i.e., we will soon release Fudge with processing) The only thing that the Fudge processing is missing is Thermal Scattering Data support and Probability tables methods such as calculated by PURR (NJOY) and PURM (AMPX). We have plans to implement both of these over the next few years.

JAEA Currently, we don't find the problem point for the open source software.

If the open source software didn't permit the modification or reformat the cross section data, some problems will be observed. Many neutron calculation code vendors add their own functions or use their own cross section data format. Since these functions and the cross section data format are secret information, it is very difficult to be published. So, they will not use and contribute the open source software.

If the open source software only prepares the typical cross section format, e.g., ACE, GENDF, WIMS and MATXS format, and permits the modification of the processing code and the cross section data format, above problem is not occurred.

CNDC Processing of the gamma production and photon-atom data; currently we rely on NJOY.

NRC KI Regarding GRUCON processing modules:

RXTXS: reconstruction cross sections from RML resonance parameters (not yet implemented);

ACE: preparation of ACE file for all representation laws of MF=6 (partially implemented, under development);

KERMA: neutron heating calculations (requires updating);

AXEXD: neutron scattering matrices in the fast energy region (requires updating).

KAERI We suggest the inclusion of the capability to deal with the ultrafine energy groups in the resonance range, which enables us to perform more accurate resonance treatment. This capability would be useful for practical reactor core design/analysis applications.