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# INDC International Nuclear Data Committee

# The New Evaluated Nuclear Data File
# Processing Capabilities

Summary Report of the Consultants' Meeting, 5-9 October 2015, IAEA, Vienna

David Brown

Brookhaven National Laboratory, Upton NY, USA

and

Andrej Trkov

IAEA Nuclear Data Section, Vienna, Austria

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# The New Evaluated Nuclear Data File Processing Capabilities

D. Brown, A. Trkov

**ABSTRACT**

A Consultants' Meeting was organized by the IAEA to review available nuclear data processing codes, discuss their status, availability, define the necessary development work and the means of implementation, and expected project-based assistance from the IAEA. As a result of this meeting a comprehensive list of activities in different laboratories related to data processing and code development was compiled, including new codes and extensions to existing codes to accommodate the newly proposed GND format for storing evaluated nuclear data. The need for a new "Code Verification Project" was expressed that would cover Doppler-broadened self-shielded and group-averaged cross sections.

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# 1. Presentations

## 1.1. Opening Remarks, A. Koning

Welcomed all present experts "working at the bottleneck of nuclear data".

## 1.2. General Introduction, A. Trkov

For many years, NJOY was the workhorse for processing nuclear data at most laboratories. Collectively we have a lot of experience working with (and debugging) NJOY. However NJOY is a "single point of failure" because many people can't access the full-featured competitors (e.g. AMPX). There are other codes that are generally available, such as PREPRO, but they are not as full-featured.

In general, member states would appreciate the availability of open source codes. This is why the status of other codes should be investigated. Are they available, and if not, can they be made available? Are there outstanding problems or missing features?

- PREPRO: Red Cullen (US) reports that it is adequate for dosimetry, but that it is missing much of what is needed for full transport calculations.
- GRUCON: From V. Sinitsa (Russia), available through IAEA for non-commercial uses; it is a comprehensive processing system but does not support some of the new features of the ENDF-6 format.
- Japan and South Korea use NJOY, JAEA is developing FRENDY.
- APMX (ORNL) is a comprehensive processing system, supporting codes developed at ORNL.
- FUDGE (LLNL) is a new development supporting the new GND format.
- NEA, IRSN use NJOY, and are developing the GAIA code system.
- CEA is developing GALILEE, and maintains the legacy code CALENDF.

## 1.3. Use of processing codes for ENDF Quality Assurance, D. Brown

Quality assurance of nuclear data used to be all 'by hand', up to as recently as ENDF/B-VI.8. Some ad-hoc automation was done by M. Herman (BNL) in the preparation for ENDF/B-VII.0. More importantly, M. Herman switched from the legacy ENDF/A – ENDF/B arrangement to a modern system running subversion as part of the GForge collaboration suite. In the run-up to ENDF/B-VII.1, NNDC automated the entire Phase I review with the ADVANCE quality assurance system.

### 1.3.1. *Advance*

ADVANCE Features
- Advance does tests automatically on every commit, but results are only published once/day due to firewall issues. Available at http://www.nndc.bnl.gov/endf/b7.dev/qa/index.html
- There are various codes called by ADVANCE including PREPRO, NJOY, NNDC codes, FUDGE, etc.
- Some of these codes have export control issues, which means the ADVANCE project repo cannot be made freely available. The system can be released without the export controlled parts.

### 1.3.2. *Issues with processing codes*

Questions raised in connection with ADVANCE (addressed during presentation):
- There is minimal thermal neutron scattering data (TNSL) checking. In principle, users would like to use NJOY, but using NJOY for thermal scattering law data is not simple;
- There are issues with processing of TNSL data: The ENDF manual is not specific enough, so processing code behavior may be undefined;

*Comment M. White (US):* processing codes are currently doing "silent fixes": changing data to get a number, but not in a transparent way. He suggests to change that and proceed as follows: 1) document where these types of fix are happening, 2) decide the "right" way to do it (i.e. make the format manual more specific if meaning of data are unclear, or change the evaluation if it contains data errors) and 3) share the decision and the solution with the full nuclear data community. Based on further discussion, this should be one of the official recommendations from this meeting.

*Another follow-up:* processing codes do sometimes need to be able to 'just produce a number', even if it means internally fixing data bugs. A suggested way forward is to enable both 'strict' and 'forgiving' modes in processing codes (library developers should be using 'strict' mode, users under deadlines may want to use 'forgiving' mode).

*Question*: Discontinuities between RRR, URR and fast region: how large a discontinuity is 'too large'? The answer is highly subjective and depends on the application.

*Question*: Can we produce angular distributions in URR (this is a topic that has come up in other groups)? At present no generally available code has this capability and the method cannot be tested.

*Discussion*: There is the risk of 'single point of failure': when only one or two codes implement a particular data processing step, cross-checking capability is limited. There is a need to have independent codes for all processing steps.

*Question*: Regarding atomic data, are there test suites available? M. White suggests a possible solution (more detail from Morgan needed).

*Question*: When bugs get reported by the child codes that Advance calls, can they be reported in a standard way? This is difficult to achieve since it would require extensive modification of legacy codes.

*Question B. Beck:* ENDF commit policy: should there be review before allowing commits? According to D. Brown we have few people making commits, so his policy is 'get it in and committed, and then iterate to fix bugs'.

*Discussion*: During lead-up to ENDF-VII.1, there was some trouble with 'commit wars', where a fix was accidentally reverted. However, as the discussion shows, this is more a question of library management and inter-lab communication instead of processing codes.

*Discussion*: A useful new capability would be a simple code to report what changed in an ENDF file at commit: less in detail than a full "diff" and tailored to ENDF needs.

**1.4. Status of Nuclear Data Processing Code at CNDC, L. Ping**

Current CNDC activities on nuclear data processing were presented. The main purpose of CNDC data processing activities is data testing of the CENDL nuclear data library and the preparation of application libraries from evaluated data. CNDC mainly uses NJOY, but PREPRO as well. CNDC is developing its own nuclear data processing code called Ruler. Modules from Ruler have been used only partially for production work.

1.4.1. *NJOY Use*
Updating NJOY99.396 to handle high energy files from JENDL high energy library.

NJOY99.396 is used to generate ACE, WIMS-D, MATXS and other data files. NJOY is hooked into the processing chain, including a code that generates AMPX formatted files.

1.4.2. *Ruler*
Ruler is written in Fortran90, and the function of Ruler is similar to NJOY.It is composed of 12 functional modules, and has an independent ENDF I/O module. The functionality of Ruler is divided into 4 parts:
- Main driver & public interface,
- data management,
- physics (RR, URR, Doppler, TST, Heating production, Multi-group ),
- interface (esp. for WIMS-D).

Ruler runs under Linux (CentOS5 & higher) and WinXP SP3 with the following capabilities:
WIMS-D/WIMSD+ format data files
Continuous energy cross sections
Resolved resonance cross section reconstruction with R-matrix limited format.

Ruler is typically much faster than NJOY as it does not use temporary files like NJOY (all inter-module communication goes through the ENDF_IO API). The Doppler broadening module is also parallelized.

KERMA is done using HEATR/NJOY or with KDC/Ruler module. At high energies, the codes behave similarly, but at low energies there are dramatic differences. KDC/Ruler is very small compared to NJOY -- the treatment of capture is very different between the two codes. It seems that the contribution from nuclear recoil is missing in Ruler. This needs further discussion.

1.4.3. *Conclusions*
CNDC uses many formats including ACE, WIMS-D and AMPX.
CNDC uses many codes downstream including MCNP, PACS, WIMS, SCALE, etc.CNDC uses a finite set of fixed group structures.

To Do:
- More testing of Ruler is needed.
- Aiming for an open source code release.
- Need for photonuclear data processing module.
- There is the intention to modify the ENDF_IO module to accept the new GND format.

**1.5. The GRUCON code package: status and projects, V. Sinitsa**

The main features of GRUCON were already presented at the WPEC-SG38 Meeting at the NEA Data Bank.

GRUCON architecture dates back to IPPE (Obninsk) with the goal to handle data in all available formats. Although the number of formats has decreased, the original goals of GRUCON are unchanged.

GRUCON contents:
- Command language for describing computation scenarios.
- Set of functional modules to perform calculations.
- System support – set of routines to interact with the system.

GRUCON input language is not straightforward, but is descriptive.

1.5.1. *GRUCON-D Release*

"GRUCON-D Computer Program Package (Demo Version)" received the Certificate of state registration; the right-holder is the Federal State Institution "National Research Center Kurchatov Institute". Although the code has been around a while, the "-D" appended to the name is more an indication that there are other components of GRUCON that could not be distributed. That said, the code is "full-featured" and runnable. The code can be requested directly from the Kurchatov Institute.

The manual is part of the release, although some parts still need further development.

There is a version of GRUCON running on the MyENDF system at the IAEA.

GRUCON distribution comes with sample data, tests, documentation and source code. Installation scripts for Windows and Linux are distributed with the main package.

Results of the GRUCON test cases were shown at the Meeting, including some verification results by comparison with the results of the PREPRO codes.

1.5.2. *GRUCON Capabilities*

GRUCON is capable of producing probability tables not just for URR, but also over the entire resonance range. Probability tables can be used efficiently in the upper part of RR energy range, where the narrow resonance approximation is valid. In the URR energy range, subgroup parameters can be obtained from cross section moments (Pade-I approxmation), or from shielded cross sections as a function of dilutions (Pade-II approximation). Benchmark results with $^{238}$U with probability tables for E > 1 keV and $^{235}$U, with E > 200 eV, are consistent with expected results to within 40 pcm. The files produced by GRUCON are noticeably smaller. In the lower part of RRR, probability parameter correlation matrices should be added to probability tables, to take into account possible correlations between parameters in consequent collisions. GRUCON provides such matrices through pointwise probability parameters in the energy groups. In other words, traditional PURR provides groupwise $P(\sigma_x/E)$, while GRUCON produces also groupwise $P(\sigma_x/\sigma_{tot},E)$.

GRUCON can also process photo-atomic data, thermal neutron scattering law data and radionuclide production data.

### 1.5.3. *Code Testing*
Recently, a GRUCON-D vs. PREPRO2015 code-to-code comparison was performed by D.L. Aldama, V. Sinitsa and A. Trkov.
- A selected set of ENDF/B-VII.1 isotopes were used as test cases. Pointwise and groupwise cross sections were compared for zero and room temperatures.
- Comparison included two GRUCON runs. In the first run, default calculation schemes and parameter values were used. In the second run, GRUCON code and input tasks were tuned to'
    - Obtained PREPRO2015 results with required accuracy 0.1%.
    - The last energy group has been excluded from consideration, due to a trivial bug in PREPRO2015 calculations that has been fixed by the author in the meantime.
    - Fe-56, cross sections above the resonance region have been broadened.
    - Fe-56, differences due to potential scattering for spin group l=2, J=7/2 were noted. The author is investigating which is the correct way to process the data..
    - Pu-239, URR interpolation scheme has been changed from cross section interpolation to parameter interpolation (in spite of of some unphysical effects that appear in the shape of the cross sections).

Disagreement in testing points requires evaluators to read the "Recommendations" sections of the ENDF manual carefully. That said, there is no mechanism to engineer away potential URR disagreements.

### 1.5.4. *Plans and projects*
- LRF=7 processing
- Expand ACE support to MF=6
- Update KERMA module
- Update transfer matrix module
- Continue cooperation with Karlsruhe Inst. Tech. on code development.

Now there is MOU to distribute GRUCON to NEA and IAEA. This is pending translation of the Russian portions of the manual and other validation activities.

## 1.6. NJOY2012 – Current Status and Future Plans, A. Kahler
This first LANL talk was a review of current NJOY and the following talk (J. Conlin) covered future plans.

### 1.6.1. *NJOY Review*
NJOY has been around for 40 years and the primary developer was Bob McFarlane. He retired in 2006, but has remained active since then.

The most widely distributed version of the code is NJOY99.

Updates are posted to a LANL website and the source code is updated through contributions by the end-users, which also allows end-users to include local patches.

Events of 9/11 caused the US to stop code sharing after NJOY99. It took many years before LANL was allowed to share NJOY again. The latest release is NJOY2012 which is the current version.

NJOY is available for a fee directly from LANL. See http://t2.lanl.gov/nis/transfer.html/. It is Export Controlled (mainly because of its commercial value).

### 1.6.2. *Current Status*

Current release is NJOY2012 which was released in December 2012. The first patch was released in August 2013 (up8). The latest patch was released in February 2015 (up50).

Current work includes:
- ACE version 2 format, especially in xsdir – expanded ZAID identifier.
- ACE plus covariance, building on work from B. Kiederowski.
- Improved LRF=7 angular distributions. There was some discussion about optimal angular resolution.
- WPEC-SG42 (TSL) improvements to THERMR & LEAPR.
- Latest CODATA constants (current release is CODATA2014, released in spring 2015). This is not a big change, but is noticeable at ENDF-6 file precision.

### 1.6.3. *Near Term Upgrade Plans*

Complete current work, as noted above.

Develop "clean code" version tentatively called NJOY2016. Need to work on LANL Technology Transfer group so that this release can be open source or at least for free. It is unclear what the current Export Control classification is based on.

A. Kahler (Skip), who is currently responsible for the official maintenance of the code will be retiring. It is foreseen that J. Conlin will take over the maintenance and code development tasks.

## 1.7. Opening NJOY for the 21$^{st}$ Century, J. Conlin

NJOY is successor to MINX ("Multigroup Interpretation of Nuclear X-Sections"), first publically released in 1977. NJOY is based on decades of experience and it is well known and trusted. However, the input "deck" format is clunky and the code is tightly coupled with the ENDF-6 format.

Side note: The name NJOY comes from taking the MINX acronym and replacing each letter with the next letter in the English alphabet in the ASCII table.

LANL has a project NJOY21 (NJOY for the 21$^{st}$ century)
- Major upgrade to NJOY2012
- Ability to use modern nuclear data formats
- Modern interaction with NJOY
- Modern code design
- Easier, faster and more flexible
- Easier to maintain
- **Backwards compatible with NJOY2012**

### 1.7.1. *Goals*

Maintain NJOY's image as a trusted and stable code
- Backwards compatibility
- Preserve capability
- Verification and Validation

Make Easier
- Build
- Verification and validation
- User interaction
- Processing
Improvements
- More flexible
- Faster
- Maintainable

### 1.7.2. *Ground up rewrite*
- C++11, with Python bindings
- Git version control
- Modern software development practices
    - Unit and integration testing
    - Issue tracking
- Backwards compatible with NJOY2012
- Open source, aiming for github release ([https://github.com/NJOY21/NJOY21.github.io](https://github.com/NJOY21/NJOY21.github.io) is reserved, but no code released is in there currently)

Such a release would enable newcomers into the nuclear data field to process and interact with nuclear data. This would also increase collaboration between LANL and the rest of the nuclear data community.

To ensure backwards compatibility, LANL is writing C++ (& Python) wrappers and a driver around legacy NJOY modules. As NJOY21 implements functionality of legacy NJOY, it will gradually replace NJOY modules. Furthermore, it will allow a command line option to trigger use of legacy NJOY code. The old NJOY scripts will continue to work with the new code even though Python interactions would be preferred.

### 1.7.3. *Current status*
The code does exist; NJOY21 is not vaporware:
- All legacy modules are available in C++
- Inputs verified for 7 NJOY modules
- Beginnings of Python interface are forming
- A native C++ ENDF6 is finished.  It is not integrated into the rest of the code.

Plans for FY16: read/write ACE, ENDF, GND files.

Wish list and other feedback is requested at njoy21@lanl.gov

*Simakov raises the question whether there are* any plans for a GUI to which *Conlin's reply is* no.

*Dunn raises the question* whether NJOY requires a SQA plan. Currently LANL management feels that NJOY does not need one. That said, it makes sense to try to formalize one's testing processes and procedures early in development rather than attempt to retrofit it on the project later.

*Mattoon points out that* GitHub has excellent sharing and feedback capability that could be taken advantage of.

*Zerkin raises the question whether there* are plans to back-port NJOY21 modules to NJOY2012. *Conlin states that* NJOY2012 is too tied to ENDF6 format to make it practical in all cases.

*White suggests that* common tasks to be carried out in connection with NJOY should be captured in the recommendations of this meeting.

*Discussion* on code comparisons and the development of simple code tests that could be used in code-to-code comparisons.

### 1.8. LLNL's Open Sourcing Philosophy and its Nuclear Data Infrastructure, B. Beck

FUDGE is LLNL's processing code. FUDGE is also used for nuclear data manipulation of all kinds. For example, LLNL evaluators have used FUDGE to generate evaluations. It is written in Python with C/C++ routines for computationally intensive tasks. Some legacy Fortran routines are included internally at LLNL but are not part of the official release.

FUDGE features:
- Read/write ENDF, ENDL (LLNL's internal format) and GND/XML
- Modify data
- Visualize data
- Checking (often finds things other codes don't and is used in ADVANCE)
- Processing, including
  - reconstructing cross sections from resonance parameters
  - linearizing data
  - heating cross sections
  - calculating average energy to outgoing particles
  - grouping data
  - calculating deterministic transfer matrices

LLNL has two potential sources of restrictions
- Classified – Nuclear data has been unclassified since 1958, therefore processing of nuclear data is unclassified
- Export control
  - Technology transfer. Want to keep other countries from obtaining certain technologies. Nuclear data and processing are exempt from this type of export control.
  - Economic advantage. Only restricts things with commercial value. Since FUDGE is available freely, it is deemed to have no commercial value.

In the past, FUDGE was released under the GPL and is available on BNL's GForge page. The most recent version supported some limited deterministic processing

The next release will be under the BSD license and all FUDGE's deterministic processing will be released.

Because LLNL uses FUDGE for programmatic work, LLNL needs to certify its contents. Therefore, LLNL will maintain the FUDGE repository but will welcome feedback and input. LLNL will review all input and requests, and if deemed appropriate, they will be added to FUDGE and included in the next release.

That said, LLNL may use github for FUDGE source control & collaboration. Github does have controls to limit who can commit to the project.

### 1.9. DAPI: an API for deterministic transport processing, B. Beck

*What is it?* It is a definition of functions, class members/methods, and inputs that define a common interface to deterministic processing codes.

*Why DAPI?* It would provide a common way for developers and users of process codes to easily processed data using any processing code that implements DAPI. Would also facilitate results from various processing codes.

There is need to determine basic inputs required by all processing codes (e.g. group boundaries, fluxes, Legendre orders, etc), basic quantities returned by codes (e.g. cross section and transfer matrix), and basic functionality (e.g. plotting).

Beck showed sample Python code using the proposed interface. This interface did not include any details about setting group structures, fluxes, etc.

There was substantial push back for mandating Python and a lot of questions about what the API would be.

Of course, a common API with commonly formatted error messages would make life easier for users and future developers. That said, all processing code developers would need to agree on the API and then implement it within their codes.

*Discussion*: Development of such an API was discussed in WPEC-SG38 meetings and it was felt that development should be part of a follow-up subgroup. It is unclear whether developers want only a low-level API or something at a higher level.

*Discussion*: Although there is substantial commonality in the processing done by different data centers, it is unclear whether it will stay that way in the future.

*Discussion*: How do you define a common interface? What do the users want? We need user cases (Fusion applications, isotope production/burn-up, etc.). This defines what users really need and thus what is needed in an API.

The fact that the different code projects outline their processing schemes as part of this meeting does make it much easier to identify the commonalities.

*Question:* Why not have a general GND API? But then it is not general enough.

Should this be part of a follow-up subgroup to Subgroup-38?

### 1.10.   Nuclear data processing with FUDGE and GND, C. Mattoon

FUDGE is an acronym meaning "For Updating Data and Generating Evaluations".
FUDGE is primarily in Python, with c, c++ and Fortran extensions. Originally FUDGE was written for LLNL's ENDL format (in "legacy" module). Current development focuses on Generalized Nuclear Data (GND), including the capability to translate back to ENDF6.

FUDGE handles incident neutrons, charged particles and gammas as well as FPY, atomic and thermal neutron scattering (limited). Decay data have yet to be implemented. Translation fidelity is assured through "round trip" translation, that is ENDF6 $\Rightarrow$ GND $\Rightarrow$ ENDF6.

### 1.10.1. *FUDGE capabilities*
Fudge can do resonance reconstruction, Doppler broadening, average energies and momenta, grouping (including computing transfer matrices).

Resonance reconstruction supports LRF=1,2,3, and LRF=7 with KRM=3. Reconstruction is done to a user-specified accuracy. "Styles" attribute helps to determine which data were original vs. those that were derived/reconstructed.

The resonance region reconstruction mostly agrees with results from RECENT and RECONR. $^{35}$Cl comparison with RECENT is favorable. However, $^{239}$Pu is problematic in the URR because the ENDF URR parameter interpolation rule was interpolated "properly" by FUDGE, but really FUDGE should do what RECENT does.

Also, $^{105}$Rh has inconsistent spins, ½ in RRR, 7/2 in URR. .

*Question by White*: even if these different spin assignments don't make physical sense, do FUDGE and GND need to support them in 'deprecated mode' for backwards compatibility?

Resonance region support also includes angular distributions for LRF=2,3 and LRF=7 pending. Also PURR support pending.

Doppler broadening results compare favorably with SIGMA1. Mostly, but there is a disagreement in the 1/v region of $^{239}$Pu. As the 1/v region is invariant under Doppler broadening, it should be straightforward to determine which code needs fixes.

*Follow-up:* The problem in FUDGE usage was diagnosed by Beck. The wrong extrapolation option was chosen (need to include cross section extrapolation below 1e-5 eV while heating). Possible action: improve default extrapolation behavior in FUDGE.

*Discussion*: NJOY, PREPRO and FUDGE have different approaches to the upper energy at which Doppler broadening is done. Experimentally, RRR measured at room temperature so as to do data-to-evaluation comparisons, one needs to broaden to at least room temperature. That said, for higher temperatures, higher energy portions of the cross section are affected by the Doppler broadening. All other codes stop at the RRR or the first inelastic threshold. FUDGE can go much higher since LLNL needs to support very hot targets such as at the National Ignition Facility (~100 keV temperatures). A complication happens when there is resonance structure in the fast region and presumably the cross section curves are based on room temperature. However the effect of room temperature broadening on a MeV resonance is negligible.

### 1.10.2. *C/C++ extensions in FUDGE:*
numericalFunctions:
- Add/subtract/multiply/divide xy interpolated functions
- Switch interpolation
- Integrate
- Compute moments (for energy & momentum deposition)

getTransferMatrix:
- per reaction or product
- all ENDF distribution types
- relativistic treatment for gammas
- compare to NJOY & APMX, identifying issues in all 3 codes
- thermal upscattering in development

### 1.10.3. *Other items*

For Monte-Carlo applications, much of the processing is deferred to the application code. Actually not really in the application code, rather in the MCGIDI package. MCGIDI is an API for GND for MC codes and does on-the-fly grouping.

Physics checking:
- Internal consistency (cross section sums, Q values vs. thresholds, …)
- Negative probabilities & incorrect normalizations
- Energy balance

*Discussion*: Doppler broadening smoothes out thresholds. How do you make sure you don't try a threshold check on heated data? *Answer*: tests are conditional on "Style" of data. Currently checking is only implemented for the 'evaluated' style, special checks could also be implemented for 'heated' style.

Visualization:
- plotEvals: plots cross sections, with EXFOR data & error bands
- compareCrossSections: 2 evaluations and their relative difference
- outgoing gamma spectra
- .plot()

Problems with ENDF/B-VII.1 outgoing gammas:
- $^{239}$Pu has no discrete MT=102 gammas until high energy
- $^{31}$P is just a histogram

*Discussion*: photon production data are reasonably accurate only for evaluations that S. Frankle did for oil well logging project CRADA and they only go up to 100 keV. In existing evaluations the focus was usually on neutrons.

Short term goals:
- Finalize a version of GND, establish format governance
- Finish MC API, implement deterministic API
- Expand tools to check/fix data
- Migrate LLNL data to GND

Long term goals:
- Support other institutes to migrate to GND
- Better treatment of thermal neutrons
- Multi-pole expansion for resonances for on-the-fly Doppler broadening

*Discussion*: Can FUDGE compute KERMA, recoil spectra, damage energy? *Answer*: not currently although there is a broken GND $\Rightarrow$ ACE tool that computed KERMA.

### 1.11.    Random sampling of resonance, G. Žerovnik

*Deterministic v.s. random sampling*: With random sampling, we are not tied to any particular PDF and can sample full space of input parameters, not just near some central value. The speed of convergence does not depend strongly on problem complexity.

*Code ENDSAM*: for random sampling or resonance parameters from ENDF6 format was developed. It reads RR & covariance file and produces samples of perturbed resonance files. The use lognormal or normal multivariate distributions are allowed. The code is available from the Meeting web page.

#### 1.11.1. *Background*
Normal distribution sampling is done with the Box-Muller method. This works well unless you have an inherently positive parameter e.g. resonance width or cross section. In such cases one may sample unphysical values.

To handle these values, one should use Log-normal distribution. This distribution does converge to Normal distribution when variance is small compared to distance of mean to zero. Sampling of this distribution may be done with a modification of the Box-Muller method.

Sampling for multivariate normal distributions can be handled with a straightforward generalization of the univariate cases. The covariance must be diagonalized and the favored way for doing this is the Cholesky decomposition.

For lognormal distributions, there exists mapping between the Normal and the log-Normal covariance; mapping was presented.  Also, how to handle a mixture of Normally and log-Normally distributed parameters was presented.

#### 1.11.2. *Issues*
Bounds on the log-Normal covariance were presented and are based on Normal covariance. These bounds also have implications for the correlations present in the log-normal covariance which are important but have been ignored in traditional approach. Therefore, when transforming from Normal covariance to log-normal covariance, correlation matrix from original covariance is kept

Some covariances in ENDF are not positive semidefinite. Their solution is to use Higham's method and find the nearest consistent correlation matrix using the Froebenius norm.

A log-normal distributions has a very long tail (like 1/x), so sampling may take a long time to converge. Brute force solution is just to add more samples. Weighted sampling is complicated when there are many parameters. Convergence of mean is slow, convergence of the variance is much slower still.

#### 1.11.3. *Results*
Currently, evaluated covariances in libraries are often not positive semi-definite and in some cases can't be fixed without major changes:
- In ENDF: $^{232}$Th, $^{238}$Np are in compact RR covariance format and are not fixable.
- In JEFF3.2: there are many isotopes, far beyond what is safely fixable with the Higham's method
- In JENDL4: $^{238}$Np is problematic.

List of evaluations with covariance not compatible with log-normal is very large (all have wrong correlations).

*Discussion*: Fixing matrices with Higham's method is a much more rigorous approach than what was done in ENDF/B-VII.1

*Discussion*: Sensitivity matrix approach+Normal distribution is sometimes a bad choice it seems. Reasons for this should be investigated.

Some isotopes are consistent with log-normal covariance, but once transformed are no longer positive semidefinite.

Sampling works, and UQ can be done with ENDSAM

## 1.12. AMPX Overview and Modernization Status, M. Dunn

### 1.12.1. *Background*
AMPX and SCALE developers are part of the ORNL Reactor and Nuclear Systems Division (RNSD). AMPX is developed and maintained by the Nuclear Data and Criticality Safety (NDCS) Group within RNSD. Mike Dunn leads the ORNL NDCS Group, and Doro Wiarda is the lead developer for AMPX. AMPX is primarily used to provide nuclear data libraries for SCALE, and the SCALE project is managed by B. Rearden. The ORNL nuclear data effort, including differential measurements and evaluation effort is tightly coupled with the modeling and simulation (M&S) efforts at ORNL. As a result, the ORNL M&S effort can respond to emerging nuclear data needs to address nuclear application analysis needs.

AMPX has been developed for ~40 years and is independent of any other nuclear data processing code chains. AMPX has a broad range of processing capabilities (e.g.., RRR, URR reconstruction, probability tables, Doppler broadening, grouping, etc.) that are used to produce continuous energy, multi-group, covariance, and depletion/decay libraries. The cross-section libraries produced by AMPX are typically distributed with SCALE.

Historically, AMPX has been used to routinely process ENDF/B evaluations since the 1970s. With the ENDF/B-6 format change and release of ENDF/B-VI in 1990, AMPX could no longer process ENDF files. The NRC funded ORNL to update AMPX between 1995-2002 to enable AMPX to process the ENDF-6 format. AMPX now keeps up with the ENDF format. Currently, the AMPX development and modernization effort is supported by the US Nuclear Criticality Safety Program (NCSP). Beginning in FY2016, the NRC also initiated a 3-year project to further support the AMPX modernization effort. In 2012, ORNL initiated a project to modernize AMPX in an effort to place the code package under SQA and develop/maintain the code package in accordance with modern software development and testing practices.

The newest version of AMPX will be released with SCALE6.2, and AMPX is currently available with the SCALE 6.2 beta release beginning with Beta Release 3. SCALE 6.2 will officially be released during the last quarter of 2015.

### 1.12.2. *Motivation for Modernization*
All things that are built are limited by the technical understanding of the time. Software is no different. When AMPX and SCALE were initially developed in the 1970s, the software was developed using the code practices of the era, and the software was designed for the computing

hardware at the time. With the evolution and advancement of computing systems, there is a need to update and modernize AMPX and SCALE.

The legacy AMPX framework and operation were similar to SCALE 5, including 77 separate processing modules and a host of different processing paths (depending on need) involving heavy reliance on I/O operations. Also, software testing was not integral to the development process. Many essential codes were "fragile," and there was a lot of code duplication between SCALE and AMPX. Also, AMPX was not developed in accordance with a formal SQA plan. In contrast, SCALE has been developed under a SQA plan for a number of years.

One of the key objectives of the AMPX modernization is to provide a unified and consistent development environment with SCALE, including better software practices and common platforms. As a result, the decision was made to merge AMPX with the SCALE development environment while keeping AMPX as a separate code package. Merging the development environment allows integration of AMPX and SCALE and minimizes the duplication of effort. Most importantly, routine and robust testing is performed as part of the development process. As AMPX is refactored, united tests are being added to AMPX.

### 1.12.3. *Status*

AMPX is now part of the SCALE repository and uses the same build & testing platforms but is a separate project. CMake performs the build for both SCALE and AMPX. Further, SCALE and AMPX can now share components [e.g. intermediate resonance self-shielding capability (improvement on Bondarenko self-shielding factors for reactor physics calculations).

With regard to SQA, AMPX development is now performed under the SCALE SQA Plan, and the SCALE SQA Plan is consistent with ISO9001, DOE 414.1 ORNL Standards Based Management System (SBMS) requirements for software development, and NQA-1. The SCALE and AMPX development is performed using the Kanban process, and all features/enhancements to the code package are tracked from the proposal phase through development and deployment. Also, ORNL uses FogBugz for bug & feature tracking with the SCALE and AMPX development. AMPX and SCALE use the same installer, and the software installs on Mac, Windows and Linux.

Moving to a modern continuous-integration (CI) development and testing framework has had a positive impact on the AMPX development. The improved development process has led to an improvement in the overall quality of the software and data libraries that are developed for SCALE. As an example, the AMPX modernization effort led to major fixes in AMPX removing a bias in the CE thermal scattering data libraries that were released with SCALE 6.1. As a result, the modernization effort has already had a significant impact on the AMPX development effort.

The ORNL SCALE/AMPX team has added many more nuclear data tests (>7000 fixed source transmission tests for neutron/gamma spectra data; >5000 infinite medium $k_{inf}$ tests, uncertainty assessment of covariance data) that are used to test AMPX and the nuclear data libraries that are produced by AMPX.

SCALE and AMPX are moving to "in-memory" data resources that reduce I/0 and enable sharing of data in memory. SCALE and AMPX now have an in-memory multi-group resource and are developing a similar resource for continuous energy data. In addition, ORNL is now working on code improvements to allow AMPX to be ready for the new ENDF/B nuclear data format transition. They will develop a local API to present XML data to AMPX and other SCALE codes.

ORNL has a desire to get AMPX exempted from US Export Control (EC) requirements, and ORNL will be working to obtain an EC exemption.

At the conclusion of the presentation, ORNL reviewed their responses to the IAEA CM nuclear data processing questionnaire.

*Discussion*: If AMPX is exempted from Export Control, will it also be open sourced? *Answer*: No, but it will still be available through RSICC.

*Discussion*: Are there capabilities to be added? *Answer*: Covariance formats MF35 & 40.

*Discussion*: How does AMPX generate probability tables? *Answer*: AMPX uses a Monte Carlo approach to calculate probability tables in the unresolved resonance region. Specifically, AMPX computes MC realizations of resonances at reference energies. The procedure also includes statistical checks to ensure convergence of the probability table generation. Furthermore, the probability table generation process is independent of the traditional "ladder" approach that was developed by Levitt and currently implemented in NJOY.

## 1.13. An alternative approach to creating ACE data files for use in Monte Carlo codes, A. Trkov, D.E. Cullen

Currently most application libraries are made with NJOY, so this presents a potential single mode of failure. Furthermore, there is a strong desire in Member States to have access to open source processing capabilities. With this background the calculations described below were performed.

PREPRO can produce multi-band parameters for self-shielding in contrast to the probability tables created by NJOY. So, can multi-band treatments replace the probability table treatment in an ACE file?

Preconditions: we cannot change MCNP and criticality calculations must remain unchanged.

### 1.13.1. *Procedure*
1. Calculate self-shielded cross sections with PURR
2. Convert cross sections to two-band parameters with URDO code
3. Replace probability tables with multiband parameters
4. Proceed with NJOY to create an ACE file.

### 1.13.2. *Testing criteria*
- Selection of Benchmarks sensitive to capture and fission of $^{235}$U and $^{238}$U.
- Benchmarks sensitive to $^{238}$U capture in 10-20 keV range (list provided by O. Cabellos).
- Availability MCNP inputs.

As a reference case we used:
a) Processing with NJOY only for $^{235}$U and $^{238}$U
b) same but with "no self-shielding".

Both of these sets of results were compared with the version using the multi-band treatment.

### 1.13.3. *Results*
Sensitivity of benchmarks to self-shielding in the URR is clear: with no self-shielding, benchmark results sometimes change by over 1000 pcm. The difference between probability tables and

multiband parameters was less than 20 pcm, compared with Monte Carlo convergence criteria of 8-3 pcm. Plots are available in the paper presented at the meeting.

It seems that we can use Red Cullen's multi-band (with only two-band) cross sections in lieu of probability tables without modifying MCNP. The resulting files are a bit smaller. The approach can also be used in deterministic codes with minimal computational overhead.

The URRDO code is available on the meeting website.

*Discussion*: The amount of size reduction from the multi-band treatment is minimal in URR, but if used in RRR, the reduction can be more than a factor of two. It would also result in much faster I/O. More importantly, this treatment will result in a vast improvement in accuracy for deterministic calculations.

*Discussion*: The benchmark SCHERZO-556 should also be useful in testing. The MCNP input is available.

*Discussion*: GRUCON is also capable of doing a multi-band treatment. This might also provide a way of cross checking Red Cullen's implementation in URRDO.

## 1.14. Nuclear Data Processing at IRSN for Transport and Criticality Safety Calculations: GAIA Code System, W. Haeck, L. Leal

The main use of data processing at IRSN is in safety assessments and validation of neutronics simulations.

The processing code are GAIA 1.x.x (NJOY wrapper), and GAIA 2; The transport code is MORET5 of VESTA; Sensitivity codes are MACSENS and BERING.

GAIA 1.x.x is a wrapper around NJOY99 & NJOY2012 and it is the current workhorse. It makes PENDF and ACE files.

GAIA 2 is under development.
- Use as standalone or integrated into other applications such as VESTA
- Capable of reading and writing ENDF, ACE, GND
- Collaborative development without "heavy" source licenses.

### 1.14.1. *Making an application library*
Processing always degrades data.

Three essential steps in preparing a library:
1. Verify library, its documentation, the methods used
2. Validate the library
3. Document everything.

Occasionally PURR tables are unphysical ($\sigma<0$) and must be fixed by hand.

Based on data in ENDF, GAIA generates the NJOY processing script.

All PostScript and log files files must be inspected by a human.

Example: fission cross section in sulphur; garbage in/garbage out.

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List of problem files was presented. All have large negative background cross sections, so messages are spurious.

### 1.14.2. *GAIA 2: A nuclear data processing software framework*
This framework should be capable of replacing the current processing capability, but also be extendable in the future. We want to be able to manipulate data outside the scope of current tools, including resonance reconstruction & heating in one step.

The key is to extract I/O from the nuclear data object in memory and routines that process object in memory.

Components of GAIA can be used as modules in another codes.

GAIA features:
- Prototyping and method development for independent capabilities at IRSN (G. Ferran, W. Haeck).
- Resonance reconstruction based on R-matrix (RRR: SLBW, MLBW, Reich-Moore and RML. The Adler-Adler formalism is also available);
- Multiple options for Doppler broadening including innovative FFT-based approach or Gaussian quadrature, but it is relatively slow;
- Calculation of angular dependent cross-section data from resonance parameters (Blatt-Biedenharn formalism).

In the future it is planned to have students working on URR, TSL and uncertainty processing.

The software was tested on benchmarks; the results for ALARM-CF-FE-SHIELD-001, n and gamma leakage from $^{252}$Cf source were presented.

*Discussion*: JEFF-3.2 22Na's PURR tables appear hopelessly broken. Other broken files are really non-errors.

*Discussion*: Will GAIA ever be available? *Answer*: Currently no.

## 1.15. Current nuclear data processing status of JAEA, K. Tada

### 1.15.1. *Reviewed responses to questionnaire*
See Appendix I

JAEA encountered bugs in NJOY2012 and developed patches which were submitted to LANL. The patches took too long to rerelease in NJOY. Because their in-house patches were not official, JAEA could not use their own patched version.

JAEA can't contribute to open source code because a) JAEA recognition may get lost and b) management might forbid it. A bigger problem is that JAEA work may be done under a non-disclosure agreement that is possibly in violation of e.g. a GPL license. A BSD license may be acceptable.

### 1.15.2. *Experience processing JENDL-4*
JENDL-4 is done by NJOY99, but some modules do not process as intended. Several evaluations stop Doppler broadening at too low an energy: $^{235}$U, $^{64}$Zn, $^{57}$Fe, etc.
The MF4 MT2 thermal scattering law process ignores the ENDF interpolation type.

NJOY99 error messages are difficult to understand.

### 1.15.3. *Enhancements for processing*
Drawing tools to compare new/old data would be useful. Also, adding text to outputs would be helpful.

*Discussion*: VIEWR has this capability, one must investigate the input format to learn how to use it.

*Discussion*: The ENDVER (IAEA) package also allows this capability, and includes comparison to experimental data.  The JANIS (NEA-OECD) package also has this possibility.

Text-based comparison is not simple.

NJOY99 & NJOY2012 make some "non-standard" data formats (PENDF & GENDF) and these are not documented.  A new format that is standardized and well documented would be helpful.

*Discussion*: The GENDF file format is detailed in the NJOY manual.  One must read the header carefully in order to determine that a given file is a GENDF file.  A. Trkov has a code that converts GENDF->ENDF

FRENDY: JAEA is developing a new processing code.  Details will be presented in ND2016. The basic approach is similar to GAIA in that it uses C++.

### 1.16.    Current Status of Nuclear Data Processing Activities at KAERI, D.H. Kim

### 1.16.1. *Introduction*
Roles of NDC, KAERI:
- Generate several kinds of XS libraries for radiation transport/depletion codes such as MCNP/MCNPX, DANTSYS, DOORS, WIMS-D, and ORIGEN.
- Disseminate them to many researchers in domestic and foreign institutions.
- Fulfil nuclear data needs for R&D activities on advanced reactors.
- Verify and validate our new evaluated data.

Nuclear Data Processing Activities at KAERI:
- No complete local ND processing code package is available.
- NJOY99, NJOY2012, ERRORJ, AMPX, PREPRO are used.
- Auxiliary tools were developed to ease NJOY processing and generate unique XS libraries for own transport/depletion codes.

### 1.16.2. *ACE-Format Library*
KAERI/NDC (KN)-Series of ACE Libraries
- The library was generated for MCNP/MCNPX and McCARD codes; the latter is a Monte Carlo transport code developed in SNU (Seoul National University).
- The codes were applied to various reactor developments such as KALIMER, SMART, VHTR and research reactors.
- KAERI/NDC is renewing their website:  http://atom.kaeri.re.kr
- All the application libraries will be posted on the website.

Multi-Temperature ACE Libraries
- Reaction XS and thermal scattering libraries at certain temperatures are available upon request.
- They are used for reactivity coefficients analysis for VHTR and research reactors.
- They are also used for the analysis of the Cold neutron facility at the Hanaro research reactor.

On-The-Fly Doppler Broadening
- Traditional XS treatments for precise temperature analyses requires a large amount of memory.
- On-the-fly DB based on Leal-Hwang DB and SIGMA1 Kernal Broadening methods has been implemented in McCARD and tested.

NJOY runs are be orchestrated by auxiliary tools ANJOYMC and NIM.

### 1.16.3. *MATXS-Format Library*
Shielding Libraries, KASHIL
- For DANTSYS & DOORS
- Processed by NJOY97/NJOY99 at several temperatures
- Applied to various reactor shielding calculations

Fast Reactor Libraries, KAFAX
- For DANTSYS
- Processed by NJOY94/NJOY99 at several temperatures
- Weighting function of KALIMER-150 core flux
- Applied to various fast reactor analyses (KALIMER)
- Supplement KAFAX library through ultrafine energy group XS treatment and self-shielded XS treatment in URR

ISOTXS-Format microscopic XS Libraries
- For MUST (Multi-group Unstructured geometry $S_N$ Transport) code
- Generated from TRANSX post-processing of KASHIL libraries at various temperatures

### 1.16.4. *Covariance Data Library*
COVFIL-formatted covariance libraries for DANTSYS/SUSD3D & others.

### 1.16.5. *PWR Core Analysis Code Library*
Multi-Group Library Generation Scheme for PWR Core Analysis
- Whole core analysis transport code DeCART
- Lattice transport codes LIBERTE & KARMA
- Application to PWR & SMART reactors

Another Scheme from Seoul National University
- Whole core transport code nTRACER
- Application to PWR & SMART reactors

### 1.16.6. *Nuclear Decay & FP Yield Library*
- For SCALE-6.1.3
- Burnup/depletion calculation by ORIGEN-S
- In-house processing tool
- Application to decay heat estimation after a fission event

Evaluated decay data with mass chains of 72 & 144 in collaboration with BNL/NNDC.

Evaluated own FP yield data of $^{235,238}$U & $^{239}$Pu.

### 1.16.7. *Suggestion*
Inclusion of capability to deal with ultrafine energy groups in RR, which enables us to perform more accurate RR treatment and is useful for practical reactor core design/analysis

*Discussion*: NJOY2012 uses dynamic memory allocation and can therefore handle the fine group structures with 10,000 groups, but its use is doubtful for the ultrafine group structures with more than 100,000.

*Discussion*: How do you validate the MATXS data as previous experience with FENDL library revealed "surprises". *Answer*: Validating with benchmarks taken from ICSBEP and SINBAD.

## 1.17. Building Enhanced Nuclear Data Services at the Data Bank, F. Michel-Sendis
(The talk is being presented at WONDER2015, concurrently with this meeting)

Also have ability to use pre-generated sensitivities to estimate the changes a particular change to an evaluation will bring to a benchmark calculation. These are used by NDAST tool.

## 1.18. MyENDF, web tool for ENDF evaluators, V. Zerkin
NDS web server applications
- MyPlot plotting with zvview (2009)
- MyEXFOR uploading system for EXFOR (2010)
- MyENDF uploading system for ENDF (2010-2015)
- MyENSDF uploading system for ENSDF (2011-2015)
- EMPIRE-3.1 (2013)

All the above allow the user to upload and test their own data without the pain of installing and learning how to run all the obscure nuclear data processing codes.

### 1.18.1. *MyENDF*
- Checking & verification codes
- Re-formatting
- Endf2gnd using FUDGE
- PREPRO2015
- ENDVER
- GRUCON

In MyENDF, you have control over the inputs for each code, although it attempts to make an educated guess for inputs via pre-loaded examples. Error messages are parsed by MyENDF using experts' knowledge to decide if particular message was important or not. The running codes can be interrupted either by the user or when the timeout counter is expired. Input files, output files generated by the codes, terminal and error output are presented to the user as a list of files with links, which can be displayed via the user's Web browser as plain text, XML, html, PS, PDF and ZVView files.

MyENDF is available at http://www-nds.iaea.org/exfor/myendf.htm

1.18.2. *Integrating MyENDF with other web-systems*
MyENDF presents the structure of user's ENDF file and offers a search of similar data via EXFOR-ENDF database retrieval system. MyENDF can accept data from users' input form, and also from other web-applications, in particular – from Empire-on-web.

1.18.3. *Empire-on-web*
EMPIRE now has a similar interface to MyENDF. Users uploading their input file, can run the three following codes:
- EMPIRE-3.1
- Formatting
- Add resonances

Users can send ENDF data to MyENDF system for further testing, processing and comparing with other evaluated and experimental data.

1.18.4. *Future*
There is not yet a clear policy for guidance from the IAEA about the future of this type of online tools (i.e. web server calculations).

*Discussion*: Most users want simple web interface like this. Many power users still need to write their own control scripts. *Answer*: MyENDF can jump-start the process by getting an initial input or control script file.

*Discussion*: Would the webapp obviate the need to a common API (e.g. DAPI)? *Answer*: Maybe for some users, but not for all users.

*Discussion*: A. Trkov showed differences between MATX & ENDF formatted data uncovered during FENDL file validation. $^{19}$F for instance clearly shows a processing problem, but the source of the problem has not been identified yet.

## 2. Recommendations

### 2.1 Get an overview of currently available processing capabilities.
    a. Write a brief discussion of user cases on which the list of needed processing capabilities may be based. This can then be mapped onto the capabilities of the various processing codes and allow to identify gaps. Cases of interest:
        i. criticality safety,
        ii. burn-up (including depletion/decay on isotope inventory and reactivity effects),
        iii. detector response (including gamma lines & correlated emission, for safeguards and global security),
        iv. heat deposition (prompt and delayed),
        v. isotope production,
        vi. radiation damage,
        vii. reactor (lattice) physics (including power distribution and accident analysis, for safeguards and nuclear energy),
        viii. radiation shielding (both earth and spaced-based radiation),
        ix. dose calculations (for health physics and medical applications),
        x. dosimetry,
        xi. design and operation of spallation neutron sources,
        xii. nuclear fusion.

*b.* Generate a list of codes and their capabilities and state where improvements are most urgently needed (in terms of methods, code availability, etc)

      i. NJOY2012 *(Action: A. Kahler)*
      ii. AMPX *(Action: D. Wiarda)*
      iii. FUDGE *(Action: B. Beck)*
      iv. FRENDY *(Action: K. Tada)*
      v. Ruler *(Action: L. Ping)*
      vi. GRUCON *(Action: V. Sinitsa)*
      vii. CALENDF *(Action: C. Jouanne and/or F. Malvagi)*
      viii. GAIA *(Action: W. Haeck)*
      ix. PREPRO *(Action: A. Trkov)*
      x. GALILEE *(Action: C. Jouanne and/or F. Malvagi)*

*c.* These lists and a description of all processing codes (with POC) should be available on the IAEA website *(Action: A. Trkov).*

**2.2 Processing code verification and validation.**

a. As part of the code validation process establish a list of data and develop recommendations for validating the codes. This list should include:

      i. Validation of resonance reconstructed cross sections at common temperatures.
      ii. Validation of Doppler-broadened cross sections – during the FENDL validation process differences between NJOY and PREPRO were observed, similarly differences were observed between FUDGE and PREPRO during FUDGE validation exercises.
      iii. Damage cross sections.
      iv. Energy deposition/KERMA – we saw large differences between NJOY & Ruler, there are very different assumptions underlying each calculation.
      v. Transfer matrices – differences between AMPX, NJOY and FUDGE were observed.
      vi. Grouped cross sections.
      vii. Moments of angular distributions (at least $P_0$ & $P_1$, but higher moments may be better).
      viii. Covariance data – only PUFF, ERRORJ and NJOY/ERRORR can use them and PUFF can compare them, there is also preliminary support in FUDGE.
      ix. Consistency of cumulative and independent fission product yields
      x. Depletion and decay data.

b. Some of the cross comparisons of matrix data are done visually. We recommend defining a more rigorous and precise method. LLNL has used Frobenius norms to test transfer matrix differences. This method is a potential starting point.

c. IAEA Report INDC(SEC)-0107 "Guidelines for nuclear data verification and validation" (https://www.nds.iaea.org/publications/indc/indc-sec-0107/) on the IAEA website provides valuable QA recommendations for ACE and MATXS files. We recommend engaging the broader nuclear data processing community to capture and document best practices for creating nuclear data libraries. These practices can then be incorporated into an expanded version of this QA document.

d. Very simple benchmarks of generated data are needed.  For example, transport can be looked at through a 1-2 MFP slab to identify any  angular distribution problems.

## 2.3  Tools for experimental/evaluated/processed data comparison

a. We recommend the development of a "diff" tool for comparing evaluations.  This tool should not do a line-by-line comparison, rather a tool that understands the ENDF (and in the future GND) structure and can report that a specific MT/MF changed. This tool could display information deeper into the file with various command line options.

b. We recommend the continued development of general tools for plotting experimental data vs. evaluated data vs. various forms of processed data.  Janis at NEA can do this to some extent; ENDVER needs to be extended to support ORNL's BOFF, LLNL's GND and the format(s) developed as part of WPEC-SG38. These alternate formats could be converted back into ENDF for viewing in ENDVER or Janis, however native support is preferred to avoid introducing new errors during the translation.

c. Visualization tools should have the capability to convolve evaluated data with experimental response functions.  These response functions are being included in newer EXFOR compilations. However, it is not always possible -- some experiments require a high-fidelity simulation of the experimental setup. In other cases, experimental data reduction has been performed and the response function and other sources of systematic error may not be recoverable.

## 2.4  Make the 'silent fixes' of all processing code make less 'silent'

a. Processing codes need to be able to 'just produce a number', even if it means internally fixing data bugs. We suggest that codes provide both 'strict' and 'forgiving' modes (evaluators and library developers should use the 'strict' mode).

b. In the longer term
   i. it should be documented what and where these types of fix are happening,
   ii. recommendations should be made for better ways to do it (i.e. make the format manual more specific if meaning of data are unclear, or change the evaluation if it contains data errors) and
   iii. each decision and the specific solution should be shared (agreed) with the broader nuclear data community.

## 2.5  Report evaluation bugs presented in this meeting to the respective data projects

a. Web retrieval systems should have a link to the library and a mechanism to send a bug report to the data project. This may not be trivial for more obscure libraries.

b. ENDF/B-VII.1 [105]Rh: it has inconsistent spins, 1/2 in RRR, 7/2 in URR. Perhaps the new JENDL-4.0 can be used to fix the URR portion of the evaluation.  [105]Rh is important for radiochemistry. This bug was reported to ENDF/B during the course of this meeting and the tracker number is #710 *(Action: task complete).*

c. RRR covariance matrix bugs in JEFF, JENDL, and ENDF/B (see Žerovnik's talk for full listing) *(Action: D. Brown, A. Trkov).*

**2.6 Investigate further improvements to the handling of the resonance region, including multi-band treatments**

      a. The ENDF Manual needs to be adjusted to ensure that interpolation in the URR is done in a rational way. Interpolating in URR parameters rather than in cross section does not completely resolve troubles.

      b. The benchmark SCHERZO-556 should be used to test multi-band treatments. The MCNP input is available *(Action: V. Sinitsa)*.

      c. GRUCON is also capable of doing a multi-band treatment. A cross comparison between the approach presented by A. Trkov and D.E. Cullen and GRUCON should be performed.

      d. Post the ACE files for $^{235}$U and $^{238}$U with the multiband parameters on the IAEA website *(Action: A. Trkov)*.

**2.7 Assemble a list of recommended tests of evaluated data in the processing codes**

a. Our test coverage of evaluated data is reasonably complete for neutron incident data. For other evaluated data, the testing is substantially more incomplete. We have experience with neutron and charged particle data, but less experience with FPY and decay data. A list of recommended tests is needed for:

      i. Thermal Scattering Law data, including tests of material stoichiometry.

      ii. Atomic data testing currently consists of plotting cross sections and form factors, more tests are needed.

      iii. Covariance tests beyond simple positivity tests are needed.

      iv. Tests of the consistency of cumulative and independent fission product yield data are needed; it is observed that they are in disagreement.

      v. Decay. Data.

Expanded testing is needed for neutron, charged particle and photonuclear data.

b. Develop integral benchmark tests of charged particle and photonuclear data.

c. Processing codes are not data checking codes. However as a side effect of their operation they must do some limited checking. Therefore, the minimum set of tests that are expected of a processing code on a per application basis need to be defined.

d. The error messages from processing codes must be easy to understand and small descriptions of the tests be provided. Error messages reported for the same reason by different codes should have a common "tag". This simplifies searching and filtering on messages. Also, the importance of various messages must be communicated.

**2.8 Codes should be made available as far as administratively possible**

      a. Post Žerovnik's ENDSAM on the IAEA website *(Action: A. Trkov)*.

      b. Post ACELST and MXSLST on the IAEA website *(Action: A. Trkov)*.

      c. Examine whether open source release of processing codes is allowed.

      d. Investigate removing Export Control restrictions on processing codes.

**2.9 Proposal for NJOY extension.**

In NJOY, investigate whether it is capable of handling ultrafine energy groups (~$10^5$ groups) in the resolved resonance region. This would enable more accurate treatment and would be useful for reactor core design/analysis. NJOY2012, with its allocable memory should be able to handle it, but this must be verified. NJOY99 would require a patch.

**Appendix I: Responses from questionnaire**

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
- LLNL: B. Beck, Lawrence Livermore National Laboratory
- JAEA: Ken-ichi Tada, Japan Atomic Energy Agency
- CNDC: Liu Ping, China Nuclear Data Centre
- ORNL: M. Dunn, Oak Ridge National Laboratory
- IRSN: W. Haeck, Institut de Radioprotection et de Sûreté Nucléaire
- OECD-NEA: O. Cabellos, Nuclear Energy Agency, OECD
- Kurchatov: V. Sinitsa, Kurchatov Institute, Moscow, Russia
- KAERI: D.H. Kim, Korea Atomic Energy Research Institute
- LANL: J. Conlin and A.H. Kahler, Los Alamos National Laboratory

*1. 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. An 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.

LLNL    We serve LLNL nuclear data users. They require viewing, manipulation (e.g, random realizations for UQ studies using code '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 produce 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 is the publication of this cross section libraries to the calculation code users.

CNDC    Data testing of CENDL nuclear data libraries.
Preparation of application libraries from evaluated data files.

ORNL    AMPX is used to provide continuous energy, multi-group, and covariance data libraries for radiation transport and sensitivity uncertainty analysis packages.

IRSN    At IRSN, we process our nuclear data libraries for both our in-house codes and third party codes that are in use at IRSN. We use NJOY 99 and NJOY 2012 for our processing. AMPX will most likely be used in the future to prepare data libraries for SCALE, should the need arise.

NEA     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. With 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, AMPX, MATXS, ...).

K.I.    The purpose of our processing activity is the preparation and verification of pointwise, multigroup and subgroup (probabilistic) data from evaluated data files and simulating integral experiments for nuclear engineering: reactor physics, radiation shielding, neutron dosimetry, fuel handling and storage, criticality safety.

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.

LANL    To provide application data for a wide range of neutronics analysis.


2.  *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.

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

JAEA    We use the NJOY99 and the PREPRO code. Now, we also use the NJOY2012 code for 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

ORNL    Primarily, AMPX is used to provide nuclear data libraries for the SCALE radiation transport package. Also, the AMPX nuclear data libraries are provided to the DOE Consortium for Advanced Simulation of Light Water Reactors (CASL) radiation transport tools. AMPX can be used to provide data for NJOY/ACER processing to generate MCNP libraries.

AMPX, SCALE, CASL, and MCNP are subject to US Export Control laws. The ORNL-developed AMPX and SCALE packages are provided by either RSICC or the OECD/NEA Data Bank. Note that AMPX is distributed with the SCALE code package. In the future, we will be able to distribute AMPX separately from SCALE. Currently, users would request SCALE/AMPX, and the user is able to select whether they would like to install AMPX only or the entire suite of SCALE/AMPX code packages.

IRSN    We produce our data libraries for the Monte Carlo transport code MORET5 and the Monte Carlo based depletion software package VESTA (both developed at IRSN) as well as for MCNP and MCNPX. As stated above, this might be extended to SCALE in the near future.

NEA    OECD/NEA Data Bank validates processed data with MCNP (with NJOY2012) and SCALE (AMPX). Applications are tested with different Benchmarks (ICSBEP – criticality and spectral indexes, SINBAD, IRPhE, …).

K.I.    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), $C^4R/C^4P$/SIMMER (Karlsruhe Institute of Technology,KIT).
None is open source.

KAERI    We usually use 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. Except for McCARD, these Korean made codes  may not be open to the public.

LANL    MCNP (Monte Carlo continuous-energy, combinatorial geometry multi-particle transport).

PARTISN (1,2,3D multigroup deterministic transport solver) (modern progeny of DTF, ANISN and DANTSYS systems).

Codes are licensed through LANL Tech Transfer, US RSICC and NEA DB

### 3.   *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.

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.

ORNL  SCALE/AMPX CE and MG data format,

SCALE/AMPX Coverx format for covariance data,

CE: ENDF TAB1 and NJOY PENDF,

Collision kinematics can be provided in native AMPX collision kinematics format.

IRSN  For MORET5 and MCNP(X) this is the ACE format and for VESTA this is the PENDF format.

NEA  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.

K.I.  Domestic formats: BNAB, TEMBR;

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.

LANL  ACE (Monte Carlo) for MCNP,

NDI (in-house multigroup format) for PARTISN.

**4. 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

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 group 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 group structure is divided by equal lethargy width. To consider the average lethargy increase by the elastic scattering of $^{238}$U, 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 group 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.

ORNL AMPX can generate MG libraries in any desired group structure format. Primarily, AMPX is used to produce MG libraries in the 252-group and 56-group SCALE group structures. Additional details about the energy group boundaries can be provided if needed.

Also, the MG libraries are provided for different problem-dependent self-shielding needs. AMPX provides CE data that are used by the SCALE CE 1-D deterministic code CENTRM to perform problem-dependent self-shielding calculations to produce self-shielded MG libraries. Also, AMPX provides MG libraries with pre-computed Bondarenko factors for resonance self-shielding calculations in either the URR and/or the RRR if desired. Recently, AMPX has been updated to provided intermediate resonance self-shielding (IR) factors for improved reactor calculations. All of the AMPX MG libraries are generated with these factors to support resonance self-shielding calculations.

IRSN    IRSN currently does not prepare data libraries for deterministic codes (although this might be changed in the future due to our use of DRAGON and CASMO).

NEA     Continuous energy (CE) for ACE and AMPX libraries. Multi-group (MG) for SCALE.

K.I.    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.

LANL   618 group master structure with various broad group collapses for different applications


5.   *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.

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 our 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 our own nuclear data processing code.

ORNL   As noted above AMPX is subject to US Export Control laws.

IRSN　For our "industrial" applications, we have developed GAIA 1.x.x, a wrapper around NJOY 99 or NJOY 2012 that generates the NJOY input files and provides QA on the produced library files (message analysis, ptable analysis, etc.). This tool will be distributed as an executable only as part of our software distribution. GAIA actually uses an external NJOY executable and contains no component taken from NJOY. NJOY will not be included in the distribution. The user must provide his own NJOY executable for the software to work.

For the future, IRSN has started working on GAIA 2 which will become our own nuclear data processing software framework. This should work both as an independent application or integrated into other software. We are currently in the prototype and methods development stage. The working capabilities include resonance reconstruction using R-matrix theory and Doppler broadening using Fast Fourier transformations or Gauss quadrature techniques. We currently have no plans on releasing this software soon but open source distribution will be taken under consideration.

NEA　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, the JANIS tool has been developed. For Benchmarking purposes the DICE system is used. JANIS and DICE have been developed by NEA.

K.I.　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.

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.

LANL　NJOY2012 - license available on request from Los Alamos National Laboratory Tech Transfer

NJOY21 - under development, expected to be open source distributed via GitHub

## 6. *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 in all likelihood implement whatever capabilities are developed through the IAEA in our ADVANCE code, especially if these capabilities are open source. 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 to the benchmarking, e.g., comparing the cross section data library which is made by JAEA with the 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.

ORNL  ORNL would be willing to contribute to the extent permitted by the US Department of Energy.

IRSN  n/a

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

K.I.  It is not prohibited to release the GRUCON package 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.

LANL  NJOY21 — Contingent upon approval, yes.


7.  *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.

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 does not permit modification or reformatting 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 have it published. So, JAEA 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.

ORNL    NJOY, AMPX and FUDGE

IRSN    n/a

NEA    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 for processing tools (e.g. NJOY, http://www.oecd-nea.org/dbprog/njoy-links.html). Including links to official and un-official updates.

K.I.    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.

LANL    Calculation of scattering matrices for deterministic transport

Calculation of free-gas and thermal scattering matrix

'diff' for evaluations and application libraries

'compare' for comparison of processed and experimental data (though ENDVER is a good start)

**Consultants' Meeting on**

"The New Evaluated Nuclear Data File
Processing Capabilities"

IAEA Headquarters, Vienna, Austria
5 – 9 October 2015
Meeting Room MOE75

**Preliminary AGENDA**

**Monday, 5 October**

**09:00 - 09:30**      **Registration** (IAEA Registration desk, Gate 1)

**09:30 - 10:15**      **Opening Session**
- Welcoming address and Introduction – Arjan Koning
  (IAEA-NDS Section Head)
- Election of Chairman and Rapporteur
- Adoption of Agenda
- Administrative matters

**10:15 - 12:30**      **Presentations by participants (about 45 min each)**
   1. A. Trkov: General Introduction (IAEA-NDS)
   2. D. Brown: Use of processing codes for ENDF Quality Assurance, BNL-NNDC

*Coffee break as needed*

*12:30 – 14:00*      *Lunch*

**14:00 – 17:30**      **Presentations by participants (cont'd)**

   3. Liu Ping: Status of Nuclea Data Processing Code at CNDC, CIAE-CNDC
   4. V. Sinitsa: The GRUCON code package: status and projects, NRC Kurchatov Institute
   5. A. Kahler: NJOY2012 – Current Status and Future Plans, LANL
   6. J. Conlin: Opening NJOY for the 21st Century, LANL

*Coffee break as needed*

**Tuesday, 6 October**

09:00 - 12:30      **Presentations by participants (cont'd)**

   7. G. Žerovnik: Consistent sampling of resonance parameters from covariance data
      (IRMM)
   8. B. Beck:
         a) LLNL's philosophy on its open source nuclear data infrastructure
         b) Status of GND and Fudge
         c) Common API fir deterministic processing
   9. M. Dunn: Status of the AMPX Cross Section Processing System
   10. OECD/NEA Data Bank

*Coffee break as needed*

*12:30 – 14:00*      *Lunch*

14:00 – 17:30     **Presentations by participants (cont'd)**
   11. CEA: TBD
   12. L. Leal (presented by W. Haeck): Nuclear Data Processing at IRSN for Transport and Criticality Safety Calculations: GAIA Code System (IRSN)
   13. JAEA: Keichi Tada: Current nuclear data Processing status of JAEA
   14. KAERI: Current Status of Nuclear Data Processing Activities at KAERI

*Coffee break as needed*

## Wednesday, 7 October

09:00 - 12:30     Round Table Discussion

*Coffee break as needed*

*12:30 – 14:00     Lunch*

14:00 – 17:30     Drafting of the summary report on codes

*Coffee break as needed*

## Thursday, 8 October

09:00     Time for each institution to present review and feedback on the requirements document,  approximately 15 minutes per organization

- CEA Malvagi
- IRSN Haeck
- IAEA Zerkin
- LANL White
- ORNL Wiarda

10:15     Proposal regarding a style guide for specifications and for the 'canonical' style when storing and exchanging nuclear data evaluations
Conlin, 15 minutes

*10:30   Break*

10:45   First writing session. Tentative writing assignments:

- documentation', 'links' and 'product' elements:
  Conlin, Coste-Delclaux, Kahler
- 'crossSection', 'dcrossSection_dOmega' and 'dcrossSection_dOmega_dE':
  Dunn, Malvagi, Tada
- 'multiplicity' and 'fissionEnergyRelease':
  Cho, Jouanne, White
- 'resonances':
  Haeck, Mattoon, Sinitsa
- 'distributions':
  Beck, Cabellos, Wiarda

*12:30* **Lunch**

14:00 Processing code update from CEA if possible?
14:30 Feedback from first writing session

15:30 Second writing session. Tentative writing assignments:

- 'reactionProducts', 'orphanedProducts' and 'decayProducts':
  Conlin, Coste-Delclaux, Kahler
- derived data (URR probability tables, CDFs, energy deposition, etc.):
  Dunn, Malvagi, Tada
- 'reactions', 'summedReactions', 'derivedReactions', etc.:
  Cho, Jouanne, White
- 'covariances':
  Haeck, Mattoon, Sinitsa
- 'reaction', 'styles', reaction designators:
  Beck, Cabellos, Wiarda

17:00 Feedback from second writing session
17:30 Break for the day

## Friday, 9 October

09:00 Review and discussion of specifications from Thursday writing sessions.

10:00 Third writing session. Focus here will be on finishing up whatever sections were not completed on Thursday. If groups complete their section, they can either join other groups or start working on some of the remaining topics, which include:

- fission product yields
- thermal neutron scattering
- metaEvaluations'
- function definition section (MathML or similar)

11:30 Feedback from third writing session.

*12:30* **Lunch**

14:00 Review recent changes to low-level data containers (Beck) and particle database (Mattoon) includes discussion about 'vector-valued' functions with multiple dependent variables

*16:00* *Break*

16:15 Final discussion and summary
17:30 Closing of the meeting

Consultants Meeting on the

## "New Evaluated Nuclear Data File Processing Capabilities"

IAEA, Vienna, Austria
5 –9 October 2015

## LIST OF PARTICIPANTS

**CHINA**

Liu **Ping**
China Nuclear Data Center
China Institute of Atomic Energy
P.O. Box 275 (41)
102413 Beijing
Tel: + 86 10-6935-7712
E-mail: ping@ciae.ac.cn

**FRANCE**

Gilles **Noguere**
CEA/DEN Cadarache
St. Paul lez Durance 13108
Tel: + 33
E-mail: gilles.noguere@cea.fr

Mireille **Coste-Delclaux**
CEA Saclay
DEN/DM2S/SERMA
B470
91191 Gif sur Yvette Cedex
Tel: + 33 1 69 08 44 40
E-mail: mireille.coste-delclaux@cea.fr

Cedric **Jouanne**
CEA Saclay
DEN/DM2S/SERMA
Bat 470
91191 Gif sur Yvette cedex
Tel: + 33 1 6908 7556
E-mail: cedric.jouanne@cea.fr

Fausto **Malvagi**
CEA Saclay
DEN/DM2S/SERMA/LEPP
Bat 470
91191 Gif sur Yvette cedex
Tel: + 33 1 6908 8949
E-mail: fausto.malvagi@cea.fr

**FRANCE cont'd**

Wim **Haeck**
Institut de Radioprotection et de Sûreté
Nucléaire (IRSN)
31, avenue de la Division Leclerc
BP 17 – 92262 Fontenay-aux-Roses Cedex
Tel: + 33 1 58359083
E-mail: wim.haeck@irsn.fr

**JAPAN**

Ken-Ichi **Tada**
Research Group for Reactor Physics
and Standard Nuclear Code System,
Nuclear Data and Reactor Engineering Division,
Japan Atomic Energy Agency
Shirakata 2-4, Tokai-mura, Naka-gun
Ibaraki pref., 319-1195
Tel: + 8129282532
E-mail: tada.kenichi@jaea.go.jp

**KOREA**

Do Heon **Kim**
Nuclear Data Center
Korea Atomic Energy Research Institute
Daedeok-daero 989-111
Daejeon
Tel: + 82428688651
E-mail: kimdh@kaeri.re.kr

Young Sik **Cho**
Nuclear Data Evaluation Laboratory
Korea Atomic Energy Research Institute
Daedeok-daero 989-111
Daejeon
Tel: + 82428682637
E-mail: yscho@kaeri.re.kr

**RUSSIA**

Valentin **Sinitsa**
Kurchatov Nuclear Technology Complex
National Research Centre
"Kurchatov Institute"
Academic Kurchatov sq., 1
123182 Moscow
Tel: +
E-mail: Sinitsa_VV@nrcki.ru

**USA**

Albert C. **Kahler**
Los Alamos National Laboratory
Bldg. 200, Room 215
P.O. Box 1663, MS B214
Los Alamos NM 87545
Tel: + 1 505 606 2042
E-mail: akahler@lanl.gov

Michael **Dunn**
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge TN 37831
Tel: +
E-mail: dunnme@ornl.gov

David **Brown**
Brookhaven National Laboratory
Building 197 D
Upton NY 11973-5000
Tel: +
E-mail: dbrown@bnl.gov

**International Organization**

Oscar **Cabellos**
NEA Data Bank

OECD Nuclear Energy Agency
Le Seine Saint-Germain
12 boulevard des Iles
92130 Issy-Les-Moulineaux
Tel: +
E-mail: dbrown@bnl.gov

Gašper **Žerovnik**
EC-JRC-IRMM
Institute for Reference Materials
and Measurements

Retieseweg 111
2440 Geel -
Tel: +
E-mail: Gasper.zerovnik@ec.europa.eu

**IAEA**

Andrej **Trkov**
A-1400 Vienna
Tel. +43-1-2600 21712
E-mail: a.trkov@iaea.org

Viktor **Zerkin**
Tel. +43-1-2600 21714
E-mail: v.zerkin@iaea.org

Both:
International Atomic Energy Agency
Nuclear Data Section
Division of Physical and Chemical Sciences
Wagramer Strasse 5
A-1400 Vienna

**USA cont'd**

Dennis **McNabb**
Lawrence Livermore National Laboratory
P.O. Box 808
Livermore CA 94551
Tel: +
E-mail: mcnabb3@llnl.gov

Jeremy L. **Conlin**
Los Alamos National Laboratory
PO Box 1663, MS F663
Los Alamos NM 87545
Tel: +
E-mail: jlconlin@lanl.gov

Caleb **Mattoon**
Lawrence Livermore National Laboratory
7000 East Avenue
Livermore CA 94550
Tel: + 14254234204
E-mail: mattoon1@llnl.gov

Bret **Beck**
Lawrence Livermore National Laboratory
7000 East Avenue
LIVERMORE  CA 94550
Tel: + 19254236148
E-mail: beck6@llnl.gov

Doro **Wiarda**
Nuclear Science and Technology Division
Oak Ridge National Laboratory
P.O. Box 2008 MS-6171
OAK RIDGE, TN 37831-6171
TEL: + 18655169838
E-mail: wiardada@ornl.gov

Morgan **White**
Los Alamos National Laboratory
X-Computational Physics

PO Box 1663 MS F663
Los Alamos NM 87545
Tel: + 15055004862
E-mail: morgan@lanl.gov