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**NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE**

Working Party on International Nuclear Data Evaluation Co-operation

**Meeting of the WPEC Subgroup 50 on Developing an Automatically Readable,
Comprehensive and Curated Experimental Reaction Database**

Summary Record

14-15 September 2020
WebEx Meeting

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OECD/NEA Nuclear Science Committee

**Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
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SUMMARY RECORD

1. Welcome

The co-ordinators, **A. Lewis** and **D. Neudecker**, welcomed the participants (see *Appendix I*) and the WPEC Secretariat, **M. Fleming**. They outlined the mandate of the new SG50 as approved at the 31st WPEC meeting in May 2020 and the structure of the meeting, which covered a wide range of topics in order to survey the existing work and needs of the community.

2. Adoption of the agenda

An additional presentation by **A. Mattera** was added before the scope discussion lead by the monitor, **A. Koning**. The agenda (see *Appendix 2*) was otherwise adopted without modification.

3. Opening talks

3.1. Introduction and goals for WPEC SG50 kick-off meeting

A. Lewis reviewed the motivations behind the subgroup: to collaboratively develop a 3-layer database of experimental reaction data based on EXFOR that incorporates subjective and objective corrections/modifications in a fully machine-interpretable format. The large number of experts, 57 from 11 countries, the NEA and the IAEA, demonstrates that this topic is of considerable interest and this first meeting will be used to survey the potential contributions and create a more detailed programme of work for the subgroup.

3.2. EXFOR and machine readability

B. Pritychenko provided an overview of the EXFOR project, which grew out of national programmes in the US¹ (and elsewhere) before being established as an international project

¹ See, for example, <https://doi.org/10.1103/RevModPhys.19.259>, BNL-170, BNL-325

in the 1960s. EXFOR is a continually evolving project, both in terms of the actual content and the types of data that can be stored. For example, fission yield data were not originally compiled as a priority and are being added in significant quantities decades after the fact due to ongoing evaluation work.

While the EXFOR format is older than many of the common data file formats (e.g. XML, JSON, HDF5), it has always been very logically structured. Several EXFOR dictionaries are maintained that define the structure of EXFOR, including a set of keywords. Many of the contents in EXFOR compilations are fully defined to the level of numerical data and dictionary-defined terms/keywords, although EXFOR may use so-called ‘free text’ to describe additional details that are not confined by the dictionaries. These free text entries make machine interpretation challenging, even with sophisticated text-interpretation software packages.

The ultimate quality of EXFOR compilations depend on the work of the compiler and reviewers. While the IAEA and other members of the NRDC perform checks against the EXFOR format requirements and comparisons against other EXFOR and/or evaluated data, these only identify major errors and the compiler is responsible for capturing the full data provided by publications and/or authors. If quantities (e.g. additional uncertainty sources) are not provided in the publications or the authors, they will not be in EXFOR and over time it becomes increasingly less likely that they could be introduced in a revised entry. In some cases, authors may provide updated/corrected data that will be included in EXFOR as a superseding entry linked to the old compilation. The IAEA also maintains a feedback list where errors are identified and reviewed by the NRDC, which recompiles entries and resubmits them as either updates of the existing entries or addition of superseding entries. A notable example is the set of Maxwellian-averaged cross sections that are being revised due to corrections on the gold standard that was employed.

It was noted that the corrections included in EXFOR are exclusively those submitted by the authors and other corrections, even if they are well justified and/or accepted by the community, cannot be included. The system presented by V. Zerkin in *section 4.1* describes the correction system outside EXFOR that currently exists.

3.3. Concept for new database

S. Okumura reviewed the state-of-the-art in other worldwide databases, where machine learning algorithms are being employed to improve innovation, automation and prediction. A common feature is that fully machine-readable structure is required to take advantage of such techniques. EXFOR is a large and old database with a detailed structure, but variations exist in terms of how metadata are coded and how uncertainty identifiers are used, including non-unique Anglicisation of names. The use of free text is also a significant issue to overcome, since some essential data (including numerical data) are included in these unstructured sections. Error and uncertainty information is not always coded in precisely the way the EXFOR dictionary defines specific keywords and numbered contributions are free to specify types with free text. The layer 1 database proposed in this subgroup would be of interest to the NRDC as it may provide feedback on a novel/replacement EXFOR format, while the addition of corrections/flagging and curation are outside the work of the NRDC. Continuous engagement with the NRDC, via the US NNDC and the IAEA, will be important for SG50 to provide feedback on EXFOR development and to take advantage of insights from the EXFOR compiler community.

4. Previous work

4.1. EXFOR data correction system.

V. Zerkin described the EXFOR data correction system that was developed first in 2009 at the request of the EXFOR user community. The objective of this tool is to allow corrections to EXFOR data based on updated knowledge (e.g. new standards, decay data, abundances, etc.) and the inclusion of evaluator judgement. The data is processed from X4 to C4 and a second set of C subroutines perform corrections and output these into a modified C4 file. The main tasks implemented are the ability to modify monitors and standards, to re-normalise with updated decay data and to provide a convenient system for evaluators to directly modify data (e.g. renormalize, change units, modify uncertainties, delete subsets of the data, etc.). The workflow of this system was reviewed as well as the syntax for users to provide inputs for corrections to an entry. A simple example includes an ascension number and a set of intuitive commands such as listing two monitors with string identifiers defined in the system. An example was shown with the K. Zolotarev data on $^{64}\text{Zn}(n,p)$ cross sections, with a set of operations performed that bring the values and uncertainties more in line with other EXFOR data and evaluations. One goal of this project is to perform automatic corrections on all relevant datasets with cross section data that also contains MONIT and MON-REF keywords for monitor reactions used. Less than 10% of EXFOR contains these data and keywords. In 2014, 4507 of the 12201 such datasets had been prepared for renormalisation. In 2020, the total has risen to 15663 while 6334 have been prepared. While this represents an increase in the fraction that are prepared, the ever-increasing number of EXFOR entries has resulted in more datasets requiring preparation than 6 years ago. The manual corrections database has 6 contributions from different authors, covering 182 datasets. Several examples with plots were shown. For more information, see the following online resources:

- <https://www-nds.iaea.org/exfor/x4guide/x4corrections/x4corrections.pdf>
- https://www-nds.iaea.org/exfor/x4js/help_corr.htm
- <http://www.youtube.com/watch?v=n9P1Z134WYM>

The EXFOR format has a very clear schema that happens to be implemented in plain text with keywords. It has been processed/translated into several derivative formats such as X4+, C5, XML, JSON, and other formats. These provide different and/or additional information, such as the information from dictionaries and data in a computationally-friendly format. Some, such as C4 and C5, include only a subset (~65% and ~75%, respectively) of EXFOR. GUI and API (via curl/wget) interfaces are available, as well as direct FTP downloads. X4Lite package is a system including EXFOR SQLite relational databases for different operating systems, retrieval codes that generate datasets from EXFOR and codes that convert EXFOR into X4+, C5, C5m, JSON and XML files. This is a computational tool and database set intended for use by professional nuclear data experts and is publically available at <https://www-nds.iaea.org/cdroms/#X4Lite>.

4.2. An EXFOR JSON database and its potential for nuclear data

G. Schnabel described a new JSON database created from EXFOR, which leverages the existing EXFOR hierarchical structure and adds only the minimal characters to translate into JSON (retaining fields, content, pointers, etc.). This is generated by an exforParser

library created in R. The resulting database is trivially serialised in modern languages such as R or python and allows users to have the EXFOR database in a simple format. Several standard operations, such as the standardisation of units and merging of entries or common blocks into data require very little effort with python, for example. The source code for the `exforParser` is open source and available on a public repository on GitHub (<https://github.com/gschnabel/exforParser>). It was noted that this provides a very light-weight and ideal starting place to consider for building a more sophisticated set of databases, particularly in light of the fact that all source code is available under GPL-3.0 with the option of collaborative development between members of the subgroup. The database itself is available in MongoDB and CouchDB formats with the latter described in the GitHub project (<https://github.com/IAEA-NDS/exfor-couchdb-docker>). This is described in detail within the paper here: <https://arxiv.org/abs/1908.00209>. An interesting point for investigation would be whether certain free-text entries (e.g. uncertainty types) could be automatically interpreted through some tool. This would form an essential part of the layer 1 translation from EXFOR.

4.3. The x4i Program

D. Brown described the x4i program (<https://git.nndc.bnl.gov/dbrown/x4i>), which is a pure python interface that reads EXFOR and draws the SQLite database directly into a class system. It handles all information (including pointers) and can add uncertainties in quadrature where they are sufficiently well-defined. It is under the GPL licence and will be re-released in fully compliant Python 3.7. x4i has been used in studies including determination of co-varying datasets and has a unique module to interpret REACTION strings as a formal grammar, in the language theory sense. x4i does not have any functionality for performing corrections, but a pilot project demonstrated the ability to automatically generate covariance information from the raw EXFOR. Future work is expected to use the system of V. Zerkin to integrate corrections.

5. User needs

5.1. Needs and Contributions to a Future EXFOR

I. Thompson reviewed the use of EXFOR at LLNL, which employs the x4i tool, C4/X4 files, various NNDC/NEA/IAEA tools and other in-house interfaces. Several recommendations were made based on the collective experience of EXFOR users at LLNL. Issues/problems include incorrect units, incorrect/inaccurate plots/digitisation, final levels not recorded fully, and uncertainty sources not well described/documented. Reference documents are not always available for all EXFOR users to review (although references are provided), quality indicators are outside the scope and corrections/comments are not stored/documented in a standardised way.

Several suggestions were made regarding the operation of the NNDC and EXFOR compilation process, including checking of data before publication (as with ENSDF), use of uncertainty templates, registering expert comments, correction of compilation errors and provision of version controlled history. In discussion, it was noted that some of these features, such as the rigorous version control of EXFOR, systems for storing comments

(see *section 4.1*) and systems for recording feedback for corrections² already exist. For more information, users are requested to contact the IAEA nuclear data section. Non-neutron data is not as comprehensively stored in EXFOR, including fission product, photo-atomic and electro-atomic data. This is due to the original mission and mandate of the NRDC, whose scope has been continually reviewed and enlarged over time to include more data types. Fission products are at present an active area for compilations with all major centres providing new compilations following the release of IAEA and NNDC memos highlighting the missing entries. Other non-neutron data can be compiled but it should be noted that these are not the first priority of the NRDC. Requests for specific data should be sent to the relevant NRDC member centre or the IAEA nuclear data section.

5.2. Using Measurement Features of Experimental Data as Input for Machine Learning

D. Neudecker discussed the importance of using measurement features (e.g. detector types, samples, thicknesses, monitors, etc.) to detect correlations between datasets, better understand systematic effects and identify discrepancies or other errors. As an example, ²³⁹Pu fast fission experiments were studied with some 37 measurement features identified. Machine learning algorithms were used to cross-compare different experiment features and find unusual results. A specific case, with alpha-counting in specific experiments, helped identify and build the case for understanding outlier datasets. This can also be applied in identifying missing or underestimated uncertainties. While some of the information used in this study were easily extracted from EXFOR, it still required some two person-weeks of effort to fully compile the information for 70 datasets. Even when some data was available in EXFOR, ambiguities in the format and free text make this challenging to properly interpret. Ultimately, the information generated in this study is valuable for evaluation work and could be stored in a standardised format. By rigorously specifying the set of information that could be included in experiments we can standardise this process of supplementing EXFOR and make recommendations to the NRDC for improvements to the EXFOR dictionaries that could improve quality of the fundamental database.

5.3. Data Driven “Low-Fi” Covariances

K. Wendt discussed the common issue of missing covariance data in nuclear data libraries and the set of possible solutions that have been considered. The so-called “Low-Fi” approach was reviewed, which uses semi-empirical model code parameter variation to provide the underlying correlations that are tuned with some additional algorithms or evaluator judgement. It was noted in discussions that several works have also performed model parameter optimisation based on a range of different Bayesian methods (B/T/UMC) using differential (and/or integral) data as evidence – including curated datasets. Work using Gaussian Processes was described, where the hyperparameters of the covariance kernel are trained on EXFOR. This method uses the EXFOR data to generate covariances, but without any physics. It is entirely dependent on the assumed quality of the input EXFOR data. In comparison to other methods employing GP to complement physical model-based covariances with model defects based on differential data, this method is naturally much simpler and faster, relying only on input measurements, but can only be

² See the official NRDC feedback list: <https://www-nds.iaea.org/nrdc/error/>

applied where there is sufficient experimental data to provide coverage over the independent variables. A set of curated experimental data are also fundamentally required.

5.4. Uppsala experience of automatic data retrieval and covariance interpretation

H. Sjöstrand reviewed work done at Uppsala University to automatically interpret and modify EXFOR data. A set of rules were applied to reject measurements, increase uncertainties and provide simple experimental correlations, the last of which resulted in significant sensitivity when considering integral experiments. It was proposed that the use of integral experiments/parameters could be used to identify the uncertainty information that should be prioritised in the creation of a L2/L3 database. Examples were shown for the corrections applied to EXFOR data for multiple channels in ^{59}Ni which have been included in the IAEA system for correction reporting. Work is being done with an evaluation pipeline³ that provides complete reproducibility of the work and allows users to re-create or modify the process.

5.5. Collaboration with SG49

M. Herman discussed collaboration with and the interfaces between SG49 and SG50. The work of SG49 is focused on the evaluation of nuclear data files and relies on EXFOR data, which will naturally benefit from all of the work done in SG50. Still, current code systems have been developed using the existing X4 and derivative files (e.g. C4, C5, etc.), so efforts should be made to allow the new database to be serialised into these standard formats in the short-term. As it will be necessary to keep this work going after the SG, it is important to ensure that the process is as straightforward as possible and evaluators have a strong benefit to cost ratio. Complex ‘tax forms’ will make it difficult for SG50 to make an impact. It will also be necessary to have in mind a maintainable system that can survive after the subgroup completes its work. Several recommendations were made, including the use of GNDS and/or techniques from that project and a focus on being able to recreate covariances rather than store surfeit data that could otherwise be easily generated from less information.

5.6. Features needed for traditional evaluations at the CNDC

R. Xu reviewed the evaluation processes at CNDC, which relies upon the experimental data within EXFOR. Evaluations are verified against EXFOR and when considering EXFOR data additional information is considered, including neutron sources, flux determination, monitors and detector types. Still, determination of the quality of each EXFOR entry remains a complex process. Datasets have been developed at CNDC to record evaluator’s judgement on specific experiments in EXFOR and these may be made available to the community as part of SG50. More comments and correlated uncertainties would be very welcome and would be beneficial for CNDC work as well as other contributors to SG50.

³ See <https://inspirehep.net/literature/1814310>

6. Lessons learned

6.1. Lessons from GNDS and SG38

C. Mattoon reviewed the Generalised Nuclear Database Structure (GNDS) projects, which was launched under WPEC Subgroup 38 (SG38) and now is the subject of an ongoing WPEC Expert Group. The process for this work included a rigorous requirements development within SG38 that generated a detailed report that includes not only physical requirements but requirements for how data should be stored, interpreted and even self-documented. Following this, SG38 began the specification of GNDS and this work continues with EG-GNDS, which has released the first public version 1.9⁴ after 6 years since the start of SG38. Several recommendations were made for SG50 based on this experience:

- Follow a rigorous requirements – specifications process and expect iterations
- Generating (even rough) draft requirements/specifications is crucial for stimulating discussion/feedback and moving forward the work
- Design lower level with more flexible data containers
- Tricks used to optimise storage in GNDS introduced unnecessary complications and were eventually rejected
- Unification of evaluated data layers (raw/processed) was fundamental in GNDS and may be beneficial for SG50 to apply this to the multiple layers
- Group similar objects together where possible
- Some data containers from GNDS (resonance parameter tables, <XYs1d>, etc.) may be of interest to the work of SG50
- Metadata about experiments doesn't have a direct analogue in ENDF-6 but GNDS-2.0 (in progress) will have expanded documentation with specific metadata (not just free text) which may be a good place to start with SG50

6.2. Object-oriented databasing for nuclear data

A. Hayes presented some observations from the US NNDC's research into modernising data storage and transmission. As with ENDF and EXFOR, the ENSDF file formats are several decades old and there are ongoing efforts to consider replacement formats. At a high level, it was recommended to separate storage, which is handled with a database, from transmission, which may occur with files. This also allows the service provider to have flexibility with the database/storage solution, which a user need not be aware of (and can change without affecting services). The differences between relational and object-oriented databases were reviewed, where common technologies include 'typical' relational SQL databases and more modern NoSQL, of which document-oriented MongoDB and CouchDB are two examples. These allow database construction with more data types, including documents, images and binary data. It was noted that CouchDB is available under the open source Apache 2.0 licence while MongoDB (as of 2018) has a more complex Server Side Public License (SSPL) which is not certified by the Open Source Initiative and

⁴ See <https://doi.org/10.1787/94d5e451-en>

whose introduction resulted in removal from various Linux distributions including Debian, Fedora and RHEL. Due to issues related to this licence and the conditions on licensing of all codes being deployed in a server using MongoDB, IAEA staff have moved to CouchDB. Example database schema and the WalletCraft UI were shown, which will form the basis of the next 2020-21 Wallet Cards evaluation.

6.3. Towards a modern and comprehensive database of experimental fission yields, starting with U-238

A. Mattera reviewed work done as part of a re-evaluation project for the fission yields of ^{238}U . As a starting point for this activity, a review of all experiments were performed, which found that a large fraction or majority of independent and cumulative yield measurements were performed since the 1993 England and Rider. A detailed review using NSR provided a starting point for identification and compilation of new data. To directly integrate EXFOR data into evaluation workflows, a simpler and more intuitive JSON format was developed that could be easily serialised and integrated into calculation schemes and visualised. V. Zarkin from IAEA provided a conversion tool that generates data in this format from EXFOR. Comparisons between measurements and evaluated data were used to highlight experiments with large potential bias and/or underestimated uncertainties. Work is ongoing to include isomeric yield measurements.

6.4. EXFORTables: An analysis of EXFOR

A. Konig reviewed the motivations behind the subgroup and several of the issues that affect how users can make use of EXFOR. EXFOR is very successfully developed and maintained as part of a specific mandate to reflect data *as published* and this has an extremely high value. Ultimately, most evaluators want to be able to easily access data, have an unambiguous interpretation of these data, understand any errors or omissions without having to refer to all original publication sources (if available), utilise a carefully curated subset of high-quality data and integrate these into a variety of workflows. This would have a large impact on nuclear data evaluation, improving efficiencies and making it possible to store much of the relatively undocumented evaluator judgements in a quantitative manner. This may also enable new automated processes for nuclear data optimisation, sentiment analysis based on existing evaluations, improvement of systematic evaluation techniques and more.

As part of previous evaluation efforts, quality scoring was performed for EXFOR datasets, including 2336 nickel subentries by N. Dzysiuk, 166 proton-induced reactions from E. Alhassan and 103 other proton-induced datasets from N. Gaughan. These include entries for evaluator, year, a numerical (binary) quality value and a free text comment. Additionally, 25850 subentries were evaluated in a cross-comparison of evaluated and experimental data as part of the WPEC Subgroup 30⁵. This includes C/E values, other test statistics and a classification of quality flags that were generated for all of these subentries. Standard null hypothesis testing is also possible using the evaluated and other experimental uncertainty values with simple interpolation rules, allowing the exclusion ('Exforcism') of suspicious data that does not follow expected trends. The EXFORtables code was created as part of the T6 project to provide a straightforward local directory structure of a subset of

⁵ See [NEA/DB/DOC\(2017\)1](#)

EXFOR for evaluation, verification and validation purposes and is available for general use.

6.5. Determination of isotopes, energy range and observables

A. Koning continued his discussion and focused on the global scope of the project. Since EXFOR and all supplementary data are very large topics, a more narrow focus was proposed that should be informed by the ongoing collaborative evaluation work. The CIELO and/or INDEN isotopes for neutron-induced data were proposed and observables will then cover cross sections, nubar and PFNS, with the option of also addressing angular distributions and/or fission yields. Angular distributions would be of considerable interest for R-matrix analyses. Since there is already a wealth of template work on the first three observables, these are the most reasonable as a starting point but others should be included. Proton-induced or other non-neutron data could also be considered, although these are not the primary priority. The first steps could be to build upon the templates for specific observables to develop requirements for the initial layers and from that point format/database implementation options and methods for storing ‘subjective’ judgements will be pursued.

7. Fast region

7.1. Fast Region Total and Capture Uncertainty Templates

A. Lewis began the second day of meetings by introducing the uncertainty template work done for low energy resolution (so-called ‘fast’) transmission measurements. These are essential for supplementing the information from EXFOR with higher-level corrections. Several standard metadata (e.g. references, facility/source, detectors, sample form/composition, monitors/ratios, corrections and uncertainties) are required for these and other measurements, and specific measurement types were listed:

- Mono-energetic and TOF total cross sections
- Capture by activation analysis
- Capture by partial gamma measurement
- Capture by accelerated mass spectrometry

In each of these, energy resolution, statistical uncertainties, background correction, target density/impurities and flux normalisation were identified as common issues. Detector efficiencies, multi-scattering corrections and geometry corrections are common to activation and partial gamma measurements, while cascade modelling is specific to partial gamma measurements and accelerated mass spectrometry has its own current and AMS method ‘reproducibility’ uncertainties. Please refer to the original presentation for the bulleted lists.

Multiple-scattering corrections are a complex topic and this is not handled in a uniform way, so some indication of whether these have been included should be recorded and/or estimates should be made for potential uncertainties introduced. Where uncertainties are combined without documentation on the individual components, higher-level databases may employ systematic rules for decomposition, if relevant.

7.2. Evaluation Needs for Cross Sections

O. Iwamoto described the evaluation procedure for cross sections in the JENDL programme, where either semi-empirical, parameterised reaction models are fit to data with least square methods; least square fitting is performed without models; or resonance region parameters are fit by specific parameter analyses. In the first two cases, the provision of data with high-quality uncertainty is essential, since this forms the basis of the evaluated uncertainties in the file. As was briefly discussed in *section 6.5*, fits to angular distribution data are sensitive to the input model parameters, making it essential in the overall evaluation processes and of interest for this subgroup, along with the other data mentioned in that section. In the resonance region, details of the experimental conditions (e.g. sample properties, data correction and resolution function) are required and are often not provided in EXFOR (and/or are not in a standardised, machine-readable format). Having all of these data is essential for the re-evaluation of parameters and it would be ideally stored in a structured schema.

7.3. Suggestions for SG50 Layer-1 Templates of (n,f) Cross Sections, PFNS and Average Prompt-fission Neutron Multiplicities and Evaluation Needs

D. Neudecker reviewed the templates for three observables, based on recent work and publications, including fission cross sections, prompt fission neutron spectra and average prompt fission neutron multiplicities. For the detailed lists, please review the presentation made at the meeting.

Discussions on this topic raised several points

- Prompt fission neutron spectra
 - There is an issue with the ratio to californium, where the background of in-beam measurements and Cf measurements can vary significantly
 - Absolute ratios are not required and these can be taken as ‘shape’ measurements regardless of what is provided in the experiment
- Fission cross sections
 - Angular distributions have been important in several measurements, including n_TOF Np data
- Average prompt fission neutron multiplicities
 - Timing gates are important for background corrections
 - Manganese baths are only used in californium and may not be the priority
 - Background discrimination above thresholds for (n,2n) and (n,3n) are important to consider

In some cases these and other data can be extracted from the original references even if they are not in the EXFOR compilations.

7.4. Experimental Neutron Cross Section Measurements in the Fast Range

D. Smith provided several insights from his long and distinguished career as an experimentalist, reminding the subgroup that real experiments are far from the ideal and sterile description found in EXFOR compilations or journal publications. Experimentalists don't report 'quality' of their data but provide what auxiliary information they had available. Measurements are never mono-energetic cross sections (or equivalent), but real data are reduced as far as possible to obtain such 'observables'. For older measurements, these may not have been known/quantified and cannot be perfectly determined today. Examples include complex neutron flux spectra, three-body breakup corrections and multiple-scattering correction. In order to improve the 'trustworthiness' of data, missing corrections should be identified, taking into account what was and what should have been considered in an experiment.

7.5. Discussion on the Fast Region

The participants discussed these presentations and came to several recommendations for the work related to low-resolution 'fast' region data. A comprehensive template of corrections should be agreed that will form the basis of evaluating relevant experiments. Where corrections are missing, these are probably suitable for layer 2, while more subjective opinions would be suitable for layer 3. Several suggestions were made, including:

- Flags should be used for automatic interpretation
- Automatic and/or more objective corrections should be made before any layer-3 flags or other modifications
- Require transparent documentation/justification for these flags and provide guidelines for this documentation
- Consider a peer-review system for flags to provide additional trustworthiness of the process and output
- Where data was positively flagged, record this and provide references (e.g. journal and/or evaluation)
- Provide specific and actionable recommendations to the NRDC so that future EXFOR can better serve the evaluation community
- To allow new data to be automatically included without penalty, negative and neutral flags are required

The primary objective of this work is to store information generated in the evaluation process so that it can be reused and/or repurposed for different algorithms (e.g. ML). To make this successful, it should remain as straightforward as possible (to avoid overburdening the evaluators).

8. Resonance region

8.1. Reporting Time-Of-Flight cross section data in EXFOR

P. Schillebeeckx reviewed how results of time of flight cross section measurements are ideally reported in EXFOR, following the recommendation resulting from a consultant's meeting organised by the Nuclear Data Section of the IAEA⁶. These recommendations are based on the AGS⁷ concept, which provides a convenient method to report separately correlated and uncorrelated uncertainty components. Based on the recommended procedures transmission and reaction yield data, including full covariance information, are produced such that nuclear reaction model parameters can be derived in a least-squares adjustment to the data. In the URR the average transmission and reaction yields can only be transferred into average cross sections after correction (e.g. for self-shielding and multiple interaction). These corrections require average resonance parameters to account for resonance structures.

The NDS/IAEA recommendations include a template with the input data that are required to perform a resonance shape analysis in the resolved resonance region using codes such as REFIT and SAMMY. The input data are related to the sample properties, specifics of the TOF-spectrometer and detectors such as their TOF response functions, etc. Since the determination of reaction yields requires an additional measurement of the energy distribution of the incident neutron fluence rate, the reference or standard reaction used to determine this distribution should be specified.

Examples of transmission and capture cross section data obtained at the time-of-flight facility GELINA were given. The main systematic effects creating correlated uncertainty components were discussed. At GELINA, the uncertainties of these systematic effects are deduced from an analysis of dedicated measurements. In addition, transmission and capture cross section measurement are carried out using fixed black resonance filters to reduce bias effects to the impact of the sample on the background. For capture cross section measurements with samples that have a high neutron scattering probability, corrections due to neutron sensitivity of the detectors are required. Using fixed black resonance filters these corrections can be verified.

8.2. Nuclear Data measurements at the RPI Gaertner LINAC Center and EXFOR reporting

Y. Danon discussed the resolved resonance range measurement capabilities at RPI and their workflow from data acquisition to EXFOR compilation. He reiterated the fact that transmission and yields for specific channels are actually measured, and that a combination of data reduction and correction techniques have to be applied to generate quantities such as energy-dependent cross sections and resonance parameters. Multiple samples with different thicknesses are used and the combination of these separate measurements are used with SAMMY to generate resonance parameters. It was noted that there are EXFOR entries where a thin sample approximation is inaccurately and implicitly used to record capture

⁶ See INDC(NDS)-0647 and other materials on the IAEA website: <https://www-nds.iaea.org/index-meeting-crp/CM-RF-2013/>

⁷ See [NEA/DB/DOC\(2014\)4](https://www.iaea.org/publications/NEA/DB/DOC(2014)4)

yields as cross sections. Several additional pieces of information need to be included that are often not in published materials or theses, including TOF bins, energy resolution functions, information on all samples, covariance information and other facility details (e.g. moderator, temperatures). A discussion on the storage of resolution functions raised important points about the potential dependence on specific codes (e.g. SAMMY, REFIT) that may have licensing or maintenance issues. It could be preferable to either store detailed equations extracted from manuals or to retain frozen copies of the codes and inputs along with data to be able to recover this information in future. This touches on a wider issue of reproducibility in all analyses related to data reduction/analysis and evaluation and wherever possible, it is preferable to retain information for all steps of the analysis.

8.3. SG50: Data Formats for the URR and Covariance

J. Brown discussed the needs for the unresolved resonance range and covariances, which should prioritise reproducibility, machine readability and storing ‘As Much as Reasonably Achievable’ (AMARA). All experimental data, uncertainties and correlations should be ideally stored, in the rawest – or least reduced - form that is reasonable. In theory, a strict QA system should be in place for all reduction and other analysis, and detailed documentation/publications. The requirements are in many ways similar to the resolved range, but data is often stored in a very coarse energy discretisation for a variety of reasons. If these data could be stored with higher resolution and fluctuations – along with all necessary steps to the final averaged parameters – it would offer value for future evaluators. For covariance matrices, data can be more conveniently stored between parameters and it would be beneficial to define a standard format for this data. Some data reduction processes are performed not with more robust code packages such as SAMMY, but with in-house code snippets and scripts developed by physicists. These could be stored alongside raw data, as well as with frozen versions of specific codes used in analyses.

8.4. Resonance Region Total and Capture Uncertainty Templates

A. Lewis discussed uncertainty templates for transmission and capture measurements, which had been discussed in previous presentations and was the subject of the IAEA CM-RF-2013. This work can clearly benefit from that earlier and extensive work, co-ordinated by the IAEA, although a different format may assist in the application of these templates not only to those modern measurements by laboratories such as JRC-Geel, but also for legacy measurements with less recorded information. In the discussion, some points were raised regarding the resolution functions, fluctuation corrections and pulse-height weighting techniques. As recorded in previous sections, resolution function records could be expanded, SESH and or Monte-Carlo code modelling of samples could be retained for the understanding of fluctuations and pulse-height documentation could be improved – particularly for lower thresholds. In all cases, it is preferable to retain both the uncorrected data and correction factors to be able to re-analyse as needed.

8.5. Evaluation needs for the Resonance Region

V. Sobes discussed ongoing development of machine-learning-based wrappers for SAMMY in the resolved resonance range. The goal is to be able to reproducibly create evaluations from a set of input files and datasets. As SG50 will be ultimately preparing data for use in ML algorithms, UTK will be preparing codes to test and utilise such data and are

generated in this subgroup. One point of interest is the determination of effective weighting of measurements in previous evaluations, which may be determined through ML techniques and could form a kind of layer-3 dataset for specific legacy evaluations that could inform future work.

Collaboration between different subgroups was highlighted, with a discussion on thermal scattering, EXFOR data and SG50. It was noted that this is a specific subdomain of nuclear data that may be dealt with after the initial neutron-induced reaction observables are first piloted, although there has been substantial data added to EXFOR on this topic in recent years.

9. Any other business

The next full meeting of the subgroup will be during the week of 11-15 May 2021. This may be held in person at the NEA Headquarters but arrangements will be made for a partial or full videoconference using WebEx. Additional sub-subgroup meetings targeting requirements for specific observables/experiments, database implementation options, methods for storing 'subjective' judgements and other topics as determined by the subgroup co-ordinators will be organised on a rolling basis with the first likely during the week of 9-13 November 2020.

APPENDIX 1

List of Registrants

First Name	Last Name	Country	Note
Devin	BARRY	UNITED STATES	
Bret	BECK	UNITED STATES	
David	BROWN	UNITED STATES	
Jesse	BROWN	UNITED STATES	
Oscar	CABELLOS	SPAIN	
Roberto	CAPOTE	IAEA	
Yaron	DANON	UNITED STATES	
Michael	FLEMING	NEA	Secretariat
Daniela	FOLIGNO	NEA	
David	FOSTER	UNITED KINGDOM	
Zhigang	GE	CHINA	
Godfree	GERT	UNITED STATES	
Mark	GILBERT	UNITED KINGDOM	
Adam	HAYES	UNITED STATES	
Michal	HERMAN	UNITED STATES	
Osamu	IWAMOTO	JAPAN	
Vaibhav	JAISWAL	FRANCE	
Arjan	KONING	IAEA	Monitor
Alexander	KONOBEEV	GERMANY	
Stefan	KOPECKY	BELGIUM	
Luiz Carlos	LEAL	FRANCE	
Amanda	LEWIS	UNITED STATES	Co-ordinator
Ryan	LOREK	UNITED STATES	
Fausto	MALVAGI	FRANCE	
Andrea	MATTERA	UNITED STATES	
Caleb	MATTOON	UNITED STATES	
Elizabeth	MCCUTCHAN	UNITED STATES	
Franco	MICHEL-SENDIS	NEA	
Denise	NEUDECKER	UNITED STATES	Co-ordinator
Gustavo	NOBRE	UNITED STATES	
Gilles	NOGUÈRE	FRANCE	
Shin	OKUMURA	IAEA	
Naohiko	OTSUKA	IAEA	
Mark	PARIS	UNITED STATES	
Arjan	PLOMPEN	JRC	
Gregory	POTEL-AGUILAR	UNITED STATES	
Boris	PRITYCHENKO	UNITED STATES	
Dimitri	ROCHMAN	SWITZERLAND	
Peter	SCHILLEBEECKX	JRC	
Georg	SCHNABEL	IAEA	
Jonathan	SHIMWELL	UNITED KINGDOM	
Henrik	SJÖSTRAND	SWEDEN	
Donald	SMITH	UNITED STATES	
Vladimir	SOBES	UNITED STATES	
Alejandro	SONZOGNI	UNITED STATES	
Nicolas	SOPPERA	NEA	
Jean-Christophe	SUBLET	IAEA	
Kenya	SUYAMA	FRANCE	
Patrick	TALOU	UNITED STATES	
Ian	THOMPSON	UNITED STATES	
Olga	VILKHIVSKAYA	UNITED KINGDOM	
Matteo	VORABBI	UNITED STATES	
Jimin	WANG	CHINA	
Kyle	WENDT	UNITED STATES	
Ruirui	XU	CHINA	
Viktor	ZERKIN	IAEA	
Shaofei	ZHU	UNITED STATES	

APPENDIX 2

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)

Meeting of Subgroup 50 on Developing an Automatically Readable, Comprehensive
and Curated Experimental Reaction Database

WebEx Meeting

AGENDA

14 September 2020

Duration	PDT	CEST	JST	Title	Speaker
00:10	05:00	14:00	21:00	Introduction	A. Lewis
00:20	05:10	14:10	21:10	EXFOR and machine readability	B. Pritychenko
00:10	05:30	14:30	21:30	Philosophy of the new database	S. Okumura
00:20	05:40	14:40	21:40	EXFOR Systems	V. Zerkin
00:10	06:00	15:00	22:00	An EXFOR JSON database and its potential for nuclear data	G. Schnabel
00:10	06:10	15:10	22:10	x4i Program	D. Brown
00:10	06:20	15:20	22:20	Needs and Contributions to a future EXFOR	I. Thompson
00:10	06:30	15:30	22:30	Short break	
00:10	06:40	15:40	22:40	Using measurement features for ML of experiments	D. Neudecker
00:10	06:50	15:50	22:50	Machine-readability for LOFI covariances	K. Wendt
00:10	07:00	16:00	23:00	Uppsala experience of automatic data retrieval and covariance interpretation	H. Sjöstrand
00:10	07:10	16:10	23:10	Co-operation between SG50 and SG49	M. Herman
00:10	07:20	16:20	23:20	Features needed for traditional evaluation methods	R. Xu
00:10	07:30	16:30	23:30	Short break	
00:10	07:40	16:40	23:40	Lessons learned from GNDS	C. Mattoon
00:20	07:50	16:50	23:50	Object-oriented databasing for nuclear data	A. Hayes
00:20	08:10	17:10	00:10	Determination of scope - isotopes, energy regions, observables	A. Koning
00:30	08:30	17:30	00:30	Discussion	All
	09:00	18:00	01:00	Close day 1	

OECD/NEA Nuclear Science Committee
Working Party on International Nuclear Data Evaluation Co-operation (WPEC)

**Meeting of Subgroup 50 on Developing an Automatically Readable, Comprehensive
and Curated Experimental Reaction Database**

WebEx Meeting

AGENDA

15 September 2020

Duration	PDT	CEST	JST	Title	Speaker
00:05	05:00	14:00	21:00	Introduction	A. Lewis
00:10	05:05	14:05	21:05	Capture and total fast region templates	A. Lewis
00:10	05:15	14:15	21:15	Evaluation needs for cross sections	O. Iwamoto
00:15	05:25	14:25	21:25	(n,f), PFNS, nu-bar templates and evaluation needs	D. Neudecker
00:15	05:40	14:40	21:40	Experimental Neutron Cross Section Measurements in the Fast Range	D. Smith
00:30	05:55	14:55	21:55	Discussion on fast range	All
00:15	06:25	15:25	22:25	Short break	
00:15	06:40	15:40	22:40	Existing RR EXFOR template	P. Schillebeeckx
00:10	06:55	15:55	22:55	Providing RRR data and uncertainties	Y. Danon
00:05	07:05	16:05	23:05	Providing URR data and uncertainties	J. Brown
00:10	07:10	16:10	23:10	Resonance region uncertainty templates	A. Lewis
00:10	07:20	16:20	23:20	Evaluation needs for the RR	V. Sobes
00:30	07:30	16:30	23:30	Discussion on resonance range	All
00:10	08:00	17:00	00:00	Short break	
00:30	08:10	17:10	00:10	Finalisation on the scope of SG50	A. Lewis
00:20	08:40	17:40	00:40	Actions and AOB	A. Lewis
	09:00	18:00	01:00	Close day 2	