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NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

Working Party on International Nuclear Data Evaluation Co-operation

Meeting of the WPEC Subgroup 49 on Reproducibility in Nuclear Data Evaluation

SUMMARY RECORD

13 May 2020
WebEx remote 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-Chairs, **M. Herman** and **D. Rochman**, welcomed the participants (see ***Appendix 1***) and the WPEC Secretariat, **M. Fleming**.

2. Adoption of the agenda

The agenda as described in ***Appendix 2*** was adopted without modification.

3. Introduction

D. Rochman discussed the objectives of the subgroup, which are to develop the requirements and prototype systems for automated and information-driven evaluation, in a fully reproducible way. This should take advantage of and store (implicitly or explicitly) the expert knowledge of evaluators and fits well in a potential future with long-term, fully-remote collaboration. Detailed discussion of physics, mathematics and methods are mostly outside the scope of this activity, except in so far as they must be accommodated within the system. The system should be as portable and simple as possible and avoid unnecessary dependencies, allowing integration within a larger ecosystem of optimisation, processing and benchmarking/validation as part of specific evaluation projects (e.g. ENDF, JEFF, JENDL).

It is essential to understand what information is required as inputs (e.g. EXFOR, code inputs/instructions), why (e.g. documentation of selections/judgement) these are selected and how the system functions. Examples and test problems should be developed that can be demonstrated with different code packages.

In the previous meeting, several points were raised. A considerable amount of evaluation data is generated by model codes (often with adjustment) and much of the effort is in parameter/model/format adjustment to match experimental data. Codes such as EMPIRE and TALYS/T6 have relatively small source code with large, curated input databases. Several codes do not have (or in the near-term will not have) their authors in full-time employment. Differential and integral databases are known to have at least some data that are not accurate and must be carefully reviewed with the outputs stored[1]. Other issues include the consideration of licences, export control and security aspects of remote code execution.

The use of modern version control systems, containerisation and platforms that support automation is of clear value. In this regard, git, GitLab/Hub and containerisation technologies such as Docker have already been demonstrated. Codes and dependant resources/databases should be as compartmentalised as possible to avoid data duplication and implicit/undocumented assumptions. Code dependencies should be separated and linked via modern techniques (e.g. submodules) where possible. This work will also need to feed into a full library management and validation system (subject of ***Section 6***).

4. Status of T6 and related software

A. Koning summarised the status and plans for the T6 (TALYS and affiliated programs) suite. As a first point, he emphasised that in order for data reproducibility and automation to be possible, the full set of important historical nuclear data must be available in one convenient and machine-readable format/database. This should include both ENDF-6 evaluated data as well as EXFOR. Options for this include a full, local database (as used in TENDL) or some other API (ideally one accessible via curl). The T6/TENDL workflow was reviewed, where the input files and codes should be stored as part of a reproducible framework and all outputs could be stored as either release candidate products and/or artefacts.

TENDL-2019 was recently released and takes advantage of several updates in the T6 ecosystem, including a new TARES-1.4 for resonance formatting/analysis. The resonance range data are based on the latest ENDFB, JEFF and JENDL library data, supplemented with the 2018 edition Atlas and verified against a database of resonance integral data. Statistical resonances have been generated with the HFR methodology, using CALENDF to generate the samples based on averaged parameters provided by TALYS. Covariances are provided in both MF32 (on the parameters) and MF33 (on the cross sections) for different use cases. These are consistent with the random files generated in the TENDL process (by using the ENDSAM code).

A set of 28455 YAML(-like) EXFOR quality scoring data files have been generated from different projects, including 2336 from the evaluation work of N. Dzysiuk for nickel activation, 166 from proton-induced work by E. Alhassan and 103 from proton-induced work by N. Gaughan. 25850 were generated as part of the statistical checks developed during WPEC Subgroup 30[2].

The TALYS-2.0 code is in development, complete with a detailed tutorial, F95 with more modularity and separation of input databases. A second 'Tools for TALYS' tutorial is in development for describing the full T6 operation. Other tools including EXFORtables,

[1] On this point, the proposed WPEC Subgroup 50 will focus on the creation of derived differential databases from EXFOR that include objective and subjective corrections/flagging, while activities within WPNCS are reviewing 'quality scores' of ICSBEP benchmarks.

[2] See the report A. Koning, et al. (2010), "Quality Improvement of the EXFOR database" NEA/NSC/WPEC/DOC(2010)428 and NEA/DB/DOC(2017)1

RESONANCEtables and ENDFtables, which generate output file-drive databases and perform various checks/decompositions are all prepared at the IAEA and available by request.

5. Prototype of a ^{58}Fe EMPIRE evaluation

M. Herman showed a repository that contains the necessary inputs for a neutron-induced ^{58}Fe evaluation using EMPIRE. This includes one 'make_evaluation' script that executes EMPIRE and related code packages to generate an ENDF-6 file. It includes a set of inputs including collective levels, OMPs, resolved resonance parameters, EXFOR data in C4 format, the primary EMPIRE input file used, discrete levels and decay data. The outputs and ENDF-6 file can then be created as artefacts. This particular case[3] is based on the ENDF/B-VIII.0 evaluation with the JEFF-3.1 resonance region and a specific EMPIRE version. Several organisational points were discussed, including how to structure directories, readme content, updates/branches and releases. However, the resonance evaluations are still provided as inputs and it was agreed that a special meeting devoted to this topic should be held.

M. Fleming demonstrated an automatic pipeline process using the evaluation inputs described above and a Docker containerised version of the EMPIRE code. The EMPIRE SVN repository was processed with standard GNU tools to create a git repository including the full ~20 year history and over 5000 commits. Attached to this, a basic test environment was created to run the compilation and system tests included with EMPIRE and package this into a clean Docker image for distribution and/or use in evaluation pipelines. For a specific EMPIRE version, this gives a reproducible and portable system for any calculations. Other container technologies could also be used and may be more 'user-friendly' although Docker integrates naturally with the GitLab systems, such as the one implemented at NEA, and was selected in this case. The ENDF-6 and output files can be stored from processes run on this container and reproduced as required at a later date.

A few observations were made regarding the EMPIRE repository that are common to other code packages. Databases need rigorous version control systems and should be linked into other packages via submodules or APIs instead of duplication (which adds in maintenance issues). Any separately-developed code should also not be duplicated, but accessible through some containerisation or submoduling approach. There are strong incentives to take these actions as numerous errors have been found in deprecated versions of tools and databases that have been corrected in the master, maintained versions. While the use of older versions is of course still possible with a submoduled version control system, updates can be automatically included (or excluded) as required by the dependent software project.

6. NDS V&V Overview of GitLab project Phase 1

F. Michel-Sendis presented the motivation and plan for work using GitLab at the NEA Data Bank, which will use git repositories within GitLab to manage the JEFF project. GitLab runners will execute automated CI/CD jobs within isolated virtual machines which comply with strict security rules. The Data Bank staff will be responsible for developing and implementing the entire system for automated verification and validation (V&V) of

[3] See https://git.oecd-nea.org/science/wpec/sg49/Evaluation-inputs

file and the whole JEFF nuclear data library, while JEFF participants will upload candidate evaluated files for testing by the Data Bank and other JEFF participants, who will be able to access the files through the same system. This system is easily scalable with additional pipelines for verification and validation processes being added through additional stages and/or GitLab runners. Docker containerisation will be used to ensure reproducibility and each of these images will be built from version-controlled Dockerfiles. The images will be stored on the local GitLab registry without external access to the Docker Hub – except for official images selected by NEA IT.

D. Foligno presented the first phase of the project system, which executes a set of format compliance, 'processability' and neutron transport code serialisation using a range of ENDF utility codes, NJOY, FRENDY and Serpent. This is done for each isotope, which has its own repository. A set of Docker images are created and maintained by NEA Data Bank staff with these codes compiled within in a fully reproducible way. Artefacts are stored from select processes, such as the output ACE files or other processed data forms. A pipeline is built out of the set of these processes with a 'fail fast' design, sequentially increasing the complexity of the tests and requiring passing runs in each of the previous jobs. When files are fully tested at an isotope level, they will be clearly and automatically tagged as such in the system, allowing other users to use the files knowing that a full and clearly defined testing process has been completed. This first phase system was demonstrated with a live screen share showing example repositories and completed pipelines on a set of generated Docker images. The next phase of this project will bring together user-defined sets of files for further testing, including processes such as criticality and shielding integral benchmarks.

7. A computation EXFOR database in JSON: Migration from MongoDB to CouchDB

G. Schnabel focussed on the use of EXFOR and work to conveniently access and utilise EXFOR for more automated tasks including statistical and/or machine learning analyses. The main issue is that EXFOR is seen as a bottleneck for users who want to employ many modern, high-level languages and libraries/packages for those languages. Many nuclear data experts write their own tools to parse (parts of) EXFOR but a much more convenient method would be to translate EXFOR into a modern, hierarchical structure. EXFOR already has a hierarchy and clear set of rules that have been developed and maintained over decades, and a purposefully simple translation tool has been developed to create a more 'computational' JSON EXFOR and is stored within a docker image[4]. This includes some tasks such as standardisation of units and merger of common blocks into the data blocks. These JSON data have been stored in a NoSQL database[5]. Originally, MongoDB was used but due to the introduction of a new SSPL and removal of MongoDB from the major Linux distributions, this was migrated to CouchDB (which is under the Apache 2.0 licence). It was agreed that this is an important step towards making more sophisticated use of EXFOR data and is likely within the scope of the new subgroup proposal being considered at WPEC-31. Access to curated EXFOR data, either as a computational JSON version or C4 or otherwise, is crucial to the success of a reproducible evaluation process.

[4] See https://github.com/gschnabel/compEXFOR-docker

[5] See https://github.com/iaea-nds/exfor-couchdb-docker

8. Next meeting and any other business

It was agreed that while ‘fast’ energy OMP-based codes were already making progress and prototypes were in place, resonance parameters can only be imported from other previously generated databases (e.g. other evaluations, the *Atlas*, etc.). To truly create a reproducible evaluation, the processes that form a resolved resonance evaluation need to be stored, from raw transmission/yield measurements (or even more elementary data) to the final parameters and covariance information. A specialised meeting on this topic will be held in November 2020 and dates will be determined by October.

APPENDIX 1

List of registrants to the 13 May 2020 Meeting of Subgroup 49 on Reproducibility in Nuclear Data Evaluation

WebEx Meeting

13 May 2020

	Name	Surname	Representing	Notes
1	Vlad	AVRIGEANU	ROMANIA	
2	Marilena	AVRIGEANU	ROMANIA	
3	Eric	BAUGE	FRANCE	
4	Bret	BECK	UNITED STATES	
5	Doug	BOWEN	UNITED STATES	
6	David	BROWN	UNITED STATES	Monitor
7	Jesse	BROWN	UNITED STATES	
8	Mark	CORNOCK	UNITED KINGDOM	
9	Theresa	CUTLER	UNITED STATES	
10	Cyrille	DE SAINT JEAN	FRANCE	
11	Isabelle	DUHAMEL	FRANCE	
12	Michael	FLEMING	NEA	Secretariat
13	Daniela	FOLIGNO	NEA	
14	Tim	GAINES	UNITED KINGDOM	
15	Zhigang	GE	CHINA	
16	Wim	HAECK	UNITED STATES	
17	Michal	HERMAN	UNITED STATES	Co-chair
18	Andrew	HOLCOMB	UNITED STATES	
19	Jesson	HUTCHINSON	UNITED STATES	
20	Raphaelle	ICHOU	FRANCE	
21	Nobuyuki	IWAMOTO	JAPAN	
22	Osamu	IWAMOTO	JAPAN	Monitor
23	Arjan	KONING	IAEA	Monitor
24	Stefan	KOPECKY	JRC	
25	Luiz	LEAL	FRANCE	
26	Amanda	LEWIS	UNITED STATES	
27	Emily	LEWIS	UNITED KINGDOM	
28	Fausto	MALVAGI	FRANCE	
29	Caleb	MATTOON	UNITED STATES	
30	Elizabeth	MCCUTCHAN	UNITED STATES	
31	Franco	MICHEL-SENDIS	NEA	
32	Denise	NEUDECKER	UNITED STATES	

33	Gustavo	NOBRE	UNITED STATES	
34	Arjan	PLOMPEN	JRC	
35	Dimitri	ROCHMAN	SWITZERLAND	Co-chair
36	Evgeny	ROZHIKHIN	RUSSIA	
37	Georg	SCHNABEL	IAEA	
38	Allan	SIMPSON	UNITED KINGDOM	
39	Henrik	SJOSTRAND	SWEDEN	
40	Alejandro	SONZOGNI	UNITED STATES	
41	Ian	THOMPSON	UNITED STATES	
42	Nicholas	THOMPSON	UNITED STATES	
43	Yuan	TIAN	CHINA	
44	Olga	VILKHIVSKAYA	UNITED KINGDOM	
45	Tim	WARE	UNITED KINGDOM	
46	Dorothea	WIARDA	UNITED STATES	
47	Gasper	ZEROVNIK	BELGIUM	

APPENDIX 2

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
Meeting of Subgroup 49 on Reproducibility in Nuclear Data Evaluation

WebEx Meeting

13 May 2020

AGENDA

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:15	05:30	**14:30**	21:30	Welcome	D. Rochman, M. Herman
00:20	05:45	**14:45**	21:45	Introduction	D. Rochman
00:20	06:05	**15:05**	22:05	Comments on TALYS and T6	A. Koning
00:40	06:25	**15:25**	22:25	Prototype of a 58Fe EMPIRE evaluation	M. Herman, M. Fleming
00:30	07:05	**16:05**	23:05	Nuclear Data V&V GitLab Project at DB/NDS	F. Michel-Sendis, D. Foligno
00:20	07:35	**16:35**	23:35	A computational EXFOR database in JSON: Migration from MongoDB to CouchDB	G. Schnabel
00:25	07:55	**16:55**	23:55	Discussion	All
	08:20	**17:20**	00:20	Close	