Nuclear Energy Agency

NEA/NSC/WPEC/DOC(2019)14

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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

27 November 2019, NEA Headquarters, Boulogne-Billancourt, France

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OECD/NEA Nuclear Science Committee

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

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

NEA Headquarters Room BB10

46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

SUMMARY RECORD

1. Welcome

The Chairs, **D. Rochman** and **M. Herman** (via WebEx), welcomed the participants (see ***Appendix 1***) and the WPEC Secretariat, **M. Fleming**. The Chairs expressed their shared view on the opportunity for this subgroup to meet the needs of the nuclear data evaluation and user community by providing recommendations on how to ensure reproducibility within nuclear data programmes. This would allow many of the evaluations in nuclear data libraries to be fully traceable and allow improvements or adjustments to be made without re-engineering from limited information. This meeting serves as a preliminary opportunity to discuss the operation of different evaluation tools and workflows and run a workshop to cover computer technology issues that will be used in the activities of the subgroup.

2. Adoption of the agenda

The agenda (see ***Appendix 2***) was adopted without modification.

3. Presentations

3.1. Documenting EMPIRE-based evaluation

M. Herman reviewed the motivations behind the subgroup, how the EMPIRE code and evaluation workflow operate, and how these can be integrated within a reproducible framework. The input and output components of EMPIRE calculations were described with an example case of ^{54}Fe to provide some reference scale for the size of data, which will be essential in determining what content is retained or treated as artefact/process data. At the level of inputs, EMPIRE requires various resources common to multiple evaluation systems, such as the RIPL database and EXFOR. Some of these are parsed into secondary files such as a modified C4 and discrete level file from RIPL. Of the outputs, various quantities the compact cross section (xcs) printouts are used in subsequent post-processing and, although artefacts, may be considered for version control. Multiple Kalman filter inputs are used in the next process, requiring the xcs files from the previous calculations. Numerous outputs are generated at this stage, with varying importance for storage. However, sensitivity matrices are extremely valuable in performing adjustments to the data

without full re-execution of the evaluation workflow. In the final slides, a complete list of files for version control with EMPIRE calculations were provided.

Multiple utility codes were described, including C4SERVICE, which manipulates the experimental data within C4 to allow comparison with the evaluated data, and DeCE, which performs direct, powerful manipulation of the ENDF-6 format data.

Several comments were made regarding post-calculation adjustment/alteration, Monte-Carlo sampling/covariances, use of GNDS, resonance treatment and documentation, each of which will require detailed discussion in future meetings.

3.2. T6 – the evaluation system around TALYS

A. Koning agreed with the need for all information and knowledge in evaluations to be quantified and stored. Three utility codes were described that are aimed at a common problem for nuclear data evaluation: many of the 'databases' available today do not use effective data structures and/or they do not follow one common set of rules. The EXFORtables, ENDFtables and Resonancetables programs are a set of Fortran tools that 'dismantle' the EXFOR, ENDF and various resonance data, respectively, into a simple file structure format for use by codes within the T6 package. It was noted that structured data format (e.g. JSON, XML, HDF5) could be used to significantly increase the efficiency of file storage, serialisation and portability of such data, as well as simplifying the process of interpreting data in other code systems.

For EXFOR, reproducibility implies the storage of metadata, including quantification of the opinions through weightings or data/uncertainty adjustment. This should be integrated into machine learning systems, requiring a much more robust system than click-retrieval through graphical interfaces. Proposals for a preliminary quality database and format will be prepared as part of the work done for TENDL.

Components of the T6 system were reviewed, including the most recent releases of packages including TALYS-1.95, TASMAN-1.95, TEFAL-1.95 and sets of scripts that execute programs including the ENDF utility codes, PREPRO, NJOY and FUDGE, as well as separate scripts that parse these code outputs and identify issues for the evaluator. Investigation into the use of git-based version control and distribution is ongoing for these packages.

3.3. Experience from the T6 portable system

D. Rochman shared lessons from the process of making the T6 code package portable. This has included a significant reduction in disk usage, as well as testing across operating systems and compilers. As part of this process, the effort to integrate into a version control system has necessitated the compartmentalisation of databases, code dependencies and various utilities. Through the process of version control and use of continuous integration, this cross-platform/compiler testing will be automated, allowing the limited development resources to be more impactfully used. Various observations were shared, including the need to simplify all aspects of the software, databases and implement simple and robust checking. Ultimately, these aspects need to be handled in such a way that we can allocate our time on the truly important aspects: improving our knowledge and the quality of nuclear data.

3.4. Maintaining Nuclear Data evaluation tools – collaboration, portability and continuity – Uppsala University experience

G. Schnabel reviewed the complexity of standard nuclear data evaluation processes, which include numerous formats, algorithms, codes, languages and systems. This approach often makes it difficult to deploy, let alone collaboratively share a workflow/pipeline, creates challenges in maintaining all the systems and makes it increasingly difficult to build upon the existing processes. A system developed at Uppsala University was presented, which focuses on interfaces instead of components of the evaluation pipeline. This work has been already put into git version control and is available online at https://github.com/gschnabel. This includes a package for launching TALYS calculations over SSH on remote clusters, which has been used by collaborators in nuclear data evaluation projects. Docker containers were introduced as a method for streamlining deployment and ensuring reproducibility.

3.5. Barriers to Reproducibility and Automation

D. Brown highlighted the challenges to the effort in making nuclear data evaluations reproducible, so that these may be overcome, so far as possible, through this subgroup. The first challenge identified was the database of differential measurements, EXFOR. While an extremely large and valuable database, it is still incomplete and can be difficult to extract data from EXFOR. The former issue is the ongoing challenge and raison d'être of the NRDC and sophisticated EXFOR interfaces will be required to automate any evaluation process (as described in the presentations of M. Herman and A. Koning). The second challenge is the incomplete structure of the ENDF-6 format, although as Chair of the EG-GNDS, D. Brown is currently leading the effort to overcome this challenge. The challenge of export control on software was also raised and introduces a challenge for some evaluation pipelines if certain codes are required. It was noted that many essential codes are not export controlled and that continuous integration pipelines can be executable by only specified individuals to control permissions as required for export control agreements. Vendor lock and use of pseudo-open tools was identified as another challenge, with Docker the prime concern. No alternative container technology was known to the participants and it was agreed that processes cannot become overly reliant upon any specific technology choice, including Docker. Remote execution of processes and the inherent security concerns was also raised as a challenge. The NEA has acknowledged this for its own processes and is already engaged on solutions that are expected to be launched in early 2020. The limitations and problems within integral experiment databases were also discussed, noting that two WPNCS subgroups have been launched in the last year to address missing cross-correlation and review the quality of uncertainty quantification, in addition to the WPEC subgroups addressing this topic. Ultimately, the challenge of the subgroup will include those listed above, and the effort required to bring it all together into a coherent system.

3.6. Validation of resolved resonance region?

S. Kopecky reviewed the process of performing transmission experiments and performing the necessary data processing. These data processing steps are complex and experiment-specific, requiring potentially very different processes for ORELA and JRC-Geel measurements. To be used in evaluation, the data within EXFOR must be complemented with the information required to process it for evaluation. A discussion on the steps required

for reproducing a complete R-matrix evaluation followed, highlighting challenges for a future system that will be integrated with other evaluation tools in a complete system.

4. Workshop on the use of the NEA GitLab

The Secretariat, **M. Fleming**, gave a short workshop aimed at familiarising the participants with git version control, the GitLab system and Docker containerisation. This included hand-on training with live repositories on the NEA GitLab. The exercises began with basic instructions, introducing standard git paradigms, submoduling and software dependency. Continuous integration was introduced with practical examples and through executing and debugging pipelines. Docker was introduced and participants ran and built containers to test example code, including automated builds with Dockerfiles.

5. Next meeting and any other business

The next meeting will occur during the week of 11-15 May 2020 at the NEA Headquarters in Boulogne-Billancourt. The exact dates will be confirmed with all of the WPEC subgroup chairs and communicated in December 2020.

APPENDIX 1

List of participants to the 27 November 2019 Meeting of Subgroup 49 on Reproducibility in Nuclear Data Evaluation

	First Name	Last Name	Country	Notes
1	Erwin	ALHASSAN	SWITZERLAND	
2	Marilena	AVRIGEANU	ROMANIA	
3	Vlad	AVRIGEANU	ROMANIA	
4	David	BROWN	UNITED STATES	*Remote*
5	Oscar	CABELLOS	SPAIN	
6	Manssour	FADIL	FRANCE	
7	Luca	FIORITO	BELGIUM	
8	Michael	FLEMING	NEA	*Secretariat*
9	Michal	HERMAN	UNITED STATES	*Chair, Remote*
10	Robert	JACQMIN	FRANCE	
11	Arjan	KONING	IAEA	
12	Alexander	KONOBEEV	GERMANY	
13	Stefan	KOPECKY	BELGIUM	
14	Fausto	MALVAGI	FRANCE	
15	Robert	MILLS	UNITED KINGDOM	
16	Denise	NEUDECKER	UNITED STATES	*Remote*
17	Ray	PERRY	UNITED KINGDOM	
18	Dimitri	ROCHMAN	SWITZERLAND	*Chair*
19	Georg	SCHNABEL	AUSTRIA	
20	Allan	SIMPSON	UNITED KINGDOM	
21	Henrik	SJOSTRAND	SWEDEN	
22	Vladimir	SOBES	UNITED STATES	
23	Yuan	TIAN	CHINA	
24	Tim	WARE	UNITED KINGDOM	
25	Haicheng	WU	CHINA	
26	Xiaofei	WU	CHINA	
27	Kenji	YOKOYAMA	JAPAN	

APPENDIX 2

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

NEA Headquarters Room BB10

46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

AGENDA

SG49 - 27 November 2019 Morning Session			
09:00	09:10	Welcome and introductions	D. Rochman
09:10	09:40	Documenting EMPIRE-based evaluation	M. Herman
10:00	10:30	T6 - the evaluation system around TALYS	A. Koning
10:30	10:45	**Coffee Break**	
10:45	11:15	Experience from the T6 portable system	D. Rochman
11:15	11:45	Maintaining Nuclear Data evaluation tools - collaboration, portability and continuity - Uppsala university experience	G. Schnabel, H. Sjöstrand
11:45	12:15	Barriers to Reproducibility and Automation	D. Brown
12:15	12:30	Reproducibility in the resonance range	S. Kopecky
12:30	14:00	**Lunch Break**	

From 14:00, we will be conducting a workshop using the NEA GitLab (https://git.oecd-nea.org). **Participants must register in advance** to ensure they have accounts with the correct permissions to access the WPEC SG49 group space and carry out the exercises. Participants must come with a computer that has GNU git installed. Windows users are encouraged to find a suitable GUI client (https://git-scm.com/downloads). Those wishing to complete the Docker exercise must come with Docker installed on their machine (https://docs.docker.com/install/). If you have any questions, please contact michael.fleming@oecd-nea.org. The workshop will include six short sessions with time for questions:

- Introduction to git and the GitLab system, groups and project creation
  - Exercise: create a project space and mirror the test repository
- Tracking changes with git
  - Exercise: staging, committing and pushing to the remote
- Branches, merging and software development branch models
  - Exercise: creating branches, making merge requests and code review
- GitLab web interface tools for collaboration
  - Exercise: creating issues, git ‘blame’, statistics and user permissions
- Using built-in GitLab continuous integration and the anatomy of YAML
  - Exercise: create a valid CI configuration and test a repository
- Containerisation with Docker
  - Exercise: create a valid Dockerfile, build an image and launch inside a container

APPENDIX 3

Actions raised at the November 27 2019 Meeting of the WPEC Subgroup 49 on Reproducibility in Nuclear Data Evaluation

1. **M. Herman / M. Fleming** to implement a solution for a continuously updated EMPIRE source code git repository hosted and/or mirrored on the NEA GitLab
2. **M. Herman** to provide a practical example of an evaluation input in the NEA GitLab SG49 space
3. **D. Rochman / A. Koning** to provide links to the T6 system used for the most recent TENDL production
4. **D. Brown** to provide EXFOR API tool for use by participants
5. **A. Koning** to prepare ENDFtables, EXFORtables and Resonancetables programs for git version control and distribution to participants
6. **A. Koning** to prepare and provide a template EXFOR metadata file to store knowledge used in evaluation process
7. **S. Kopecky** to draft a list of inputs and description of the resolved resonance evaluation workflow
8. **G. Schnabel / H. Sjöstrand** to provide documentation on the containerised clusterSSH system and/or links to online resources to be posted on SG49 website
9. **M. Fleming** to provide support to participants in preparing repositories, containers and CI pipelines for nuclear data tools