Nuclear Energy Agency

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NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

Working Party on International Nuclear Data Evaluation Co-operation

Meeting of the WPEC Expert Group on the Recommended Definition of a General Nuclear Database Structure (EG-GNDS)

SUMMARY RECORD

12 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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1. Welcome

The Chair, **D. Brown**, 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. Update of the publication of GNDS-1.9

M. Fleming updated the participants on the status of the GNDS publication. Following the decision at the June 2020 meeting (NEA/NSC/WPEC/DOC(2019)2) to finalise the current specifications as version 1.9, a lengthy review was undertaken. The detailed review by EG-GNDS members and invited experts was completed in December 2019 and a draft was iterated with the NEA Central Secretariat to ensure rigorous compliance with the OECD Publication Guidelines. This resulted in a first of a kind git-managed, LaTeX report that has been finalised and accepted for publication within the OECD iLibrary[1]. As part of this process, the NEA has established new methods for reviewing such documents for publication and the subsequent GNDS publications will be streamlined. In addition to the specifications, a short policy brief will be issued by the NEA alongside other outreach activities being planned.

4. SG43 Status WPEC 2020

F. Malvagi presented an update of the work co-ordinated through Subgroup 43 on Code infrastructure to support a general nuclear database structure (GNDS). While the initial intention was for the subgroup to collectively define an API for GNDS, participants created

[1] ISBN 978-92-6490-197-1, https://www.oecd-nea.org/science/pubs/2020/7519-GNDS.pdf

several independent implementations. As of the 2020 meeting, two APIs have been published (FUDGE and GIDIplus), while several others are partially complete. Multiple organisations have already provided detailed descriptions of the checking locally performed for nuclear data files and these will be combined with the descriptions of the GNDS APIs into a final report for Subgroup 43 that is due in 2021. The participants have agreed that the overarching purpose has been to champion the implementation of tools to use GNDS and encourage its adoption by the community, which is an activity that could be integrated within the EG-GNDS.

5. Specifications vs Requirements vs ENDF-6

D. Brown reviewed the status of the current GNDS specifications against the requirements that were agreed within Subgroup 38 and the current ENDF-6 format. All of the MF and MT values within ENDF-6 have GNDS analogues and a summary of these connections has been prepared. It is not within the specifications although a format proposal may be made to propose it within a future publication. More detailed comparisons (at the LIP, LAW, etc. level) are in progress. The Subgroup 38 requirements include multiple requests that have been directly addressed in the 1.9 specifications and others are the subject of the format proposals that were made before this meeting. Some specific areas, such as fission product yields, are expected to have revised requirements proposed as part of other collaborative efforts and the EG-GNDS membership is well-placed to integrate these as and when the evaluator and/or user community clarifies their needs.

6. Atomic Data

M. G. Pia provided a detailed review of evaluated photon, atomic relaxation and electron interaction data. Modern codes such as Geant4 have relied upon libraries prepared in the 1990s that were largely the product of work done decades earlier. The main libraries (EADL/EEDL/EPDL) have benefitted from some maintenance and have been repackaged as the Electron Photon Interaction Cross Sections (EPICS)[2], but these data are not actively developed and much of the essential metadata is undocumented. Some data (e.g. Biggs' Compton profiles, Compton scattering atomic shell vacancy creation probabilities) are not stored and are required by Monte Carlo codes. These issues may be addressed by a new GNDS format that can accommodate the required data and metadata. Some examples were presented, with comments on the suitability of the E*DL data and the ENDF/GNDS formats. New requirements for these data are required to start the process for extending the GNDS specifications.

7. Fission product yields

D. Brown discussed the status of the fission product yield specifications, their shortcomings and issues that were not fully explored as part of the initial requirement preparation. He reminded the participants that real use cases often involve time-dependent solutions to the Bateman equations and that correct uncertainty propagation will require care as the full, correlated decay information is needed and is also implicitly included within the evaluation of the uncertainties of fission product yields. The matrices used to

[2] Available from https://www-nds.iaea.org/epics/

transform between independent and cumulative fission yields may also be stored, although these should be exactly reproducible from the decay data used and this would introduce a potentially unnecessary duplication. It was noted that no ENDF-6 fission yield evaluation provides this information and that several cases have been identified where inconsistencies exist between the two, suggesting that storage of this information could still be of value. Energy dependence was also raised, since the well-known evaluations have 'dummy' values associated with broad energy spectra that are not defined within the ENDF-6 format (or, potentially, anywhere). While there were many ideas put forward by the participants, it was agreed that the requirements must come from the evaluator and user community, ultimately in the form of the data that is provided for the next generation of evaluations. EG-GNDS members will continue to closely liaise with the ongoing fission product yield evaluation projects around the world to integrate these needs into future format proposals.

8. Discrete, excited and isomeric states

J-Ch. Sublet reviewed the ways that excited nuclear states are stored within the ENDF-6 format, commenting on the multiple and inconsistent ways that isomeric states and other discrete levels are identified. These have resulted in multiple bookkeeping solutions, depending on the application, which must be reconciled by users. A simple and straightforward solution was proposed: to store the Z, A, excitation energy and half-life of the state. This should be complemented by a database of the states considered with a minimum half-life (e.g. 1 ms). This may cause issues with backwards compatibility into the ENDF-6 format but in any case, it would be preferable.

9. WalletCraft – Object-oriented databasing for nuclear data

A. Hayes presented work done at BNL to improve the Nuclear Wallet Cards system, streamlining updates, synchronising with ENSDF evaluations, storing source data and metadata and providing a more rigorous version control/tracking system. CouchDB was selected for the design as it allows simple http requests and returns structured data in JSON. The schema for the entries was reviewed, with examples of level descriptions, evaluations and half-lives shown. The project is ongoing and will be used as a testbed for the future ENSDF database system.

10. Discussion on the proposals and next release

D. Brown reviewed the status of the 14 format proposals that have been included in the GNDS git system. As specified by the Procedures (NEA/NSC/WPEC/DOC(2019)1), each of these has been prepared and shared with the Expert Group membership. Each has a new branch of the repository and put forward as a merge request[3]. 12 of the 14 proposals have gone through the review process and are ready for merging into the development version of the GNDS specifications. The last two are competing options for the re-arrangement of resonance treatment. Following discussion on this point, it was agreed that further work was required to clarify the respective benefits of each proposal so that a fully-informed decision could be taken.

[3] See https://git.oecd-nea.org/science/wpec/gnds/formats/merge_requests

The next GNDS specifications will include multiple, substantial changes – including the resonance format proposal selected. It was agreed that this meeting would not approve the next GNDS specifications but continued discussions will be recorded within the merge request discussion boards. Additional, focussed meetings will be called to address these issues as required and all EG-GNDS members will be invited to participate. For the next release, the EG-GNDS agreed that the version number should be a major revision number increase to version 2.0 and this should include:

- the documentation proposal (Caleb and Dave);
- the TSL covariances proposal (Doro);
- the outstanding resonance proposal (all); and
- the background proposal discussed at the meeting (Wim, Doro, Ian).

The process to formally approve this new release will require these to go through the format proposal procedure.

11. Review of the GNDS Schema Build System

G. Godfree presented a review of the GNDS build system, which uses Python tools to create TeX from JSON files that are manually edited. This is complemented with static TeX files for various sections. The structure of these files and the use of static and dynamic TeX is not fully homogenous, making the system unnecessarily complex and more difficult to maintain. The JSON files themselves were made from XSD with an automatic translation tool, but for some time the JSON files have been manually updated without directly updating the XSD. Visualisation of the XSD and JSON node structures shows that some structure present in XSD has been lost in the conversion to JSON. It was agreed that the 'backend' system for building the GNDS specifications needs to be refactored, although this does not necessarily require any change to the specifications themselves.

12. Mandate Extension

As the GNDS specifications were published in May 2020, the mandate (see ***Appendix 3***) will now reflect the new role of the EG-GNDS in maintaining and providing periodic updates of the specifications. As WPEC Subgroup 43 will be closing after WPEC-32, it was agreed that the EG-GNDS will take over the role of championing the adoption of GNDS and organising co-operative work on the design and implementation of APIs for GNDS. This will be reviewed if and when another short-term activity may be proposed and endorsed by the parent WPEC.

13. Next meeting and any other business

The next full meeting of the EG-GNDS will be scheduled after the completion of the outstanding format proposals listed in ***Section 10***. This is expected in Q4 2020. Following this meeting, the next official EG-GNDS meeting will occur during the week of 10-14 May 2020 at the NEA Headquarters in Paris.

Appendix 1

List of Participants of the Meeting of the Expert Group on the Recommended Definition of a General Nuclear Database Structure (EG-GNDS)

#	Name	Surname	Representing	Notes
1	Bret	BECK	UNITED STATES	Member
2	Doug	BOWEN	UNITED STATES	
3	David	BROWN	UNITED STATES	Chair
4	Jeremy	CONLIN	UNITED STATES	Member
5	Mark	CORNOCK	UNITED KINGDOM	Member
6	Michael	FLEMING	NEA	Secretariat
7	Daniela	FOLIGNO	NEA	
8	Tim	GAINES	UNITED KINGDOM	
9	Godfree	GERT	UNITED STATES	
10	Wim	HAECK	UNITED STATES	Member
11	Adam	HAYES	UNITED STATES	
12	Michal	HERMAN	UNITED STATES	
13	Andrew	HOLCOMB	UNITED STATES	
14	Osamu	IWAMOTO	JAPAN	Member
15	Cedric	JOUANNE	FRANCE	Member
16	Luiz	LEAL	FRANCE	
17	Amanda	LEWIS	UNITED STATES	
18	Fausto	MALVAGI	FRANCE	Member
19	Caleb	MATTOON	UNITED STATES	Member
20	Elizabeth	MCCUTCHAN	UNITED STATES	
21	Robert	MILLS	UNITED KINGDOM	
22	Alexandru	NEGRET	ROMANIA	Member
23	Maria Grazia	PIA	ITALY	
24	Danila	ROUBTSOV	CANADA	
25	Allan	SIMPSON	UNITED KINGDOM	
26	Jean-Christophe	SUBLET	IAEA	Member
27	Pierre	TAMAGNO	FRANCE	
28	Ian	THOMPSON	UNITED STATES	Member
29	Nicholas	THOMPSON	UNITED STATES	
30	Alex	VALENTINE	UNITED KINGDOM	
31	Tim	WARE	UNITED KINGDOM	
32	Dorothea	WIARDA	UNITED STATES	Member
33	Xiaofei	WU	CHINA	

Appendix 2

Meeting of Expert Group on the Recommended Definition of a General Nuclear Database Structure (EG-GNDS)

WebEx Meeting

12 May 2020

AGENDA

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:10	03:00	**12:00**	19:00	Welcome	D. Brown
00:10	03:10	**12:10**	19:10	GNDS-1.9 publication	M. Fleming
00:15	03:20	**12:20**	19:20	API status / SG43	F. Malvagi
00:15	03:35	**12:35**	19:35	Specifications vs requirements / ENDF-6	D. Brown
00:15	03:50	**12:50**	19:50	Atomic data	M.G. Pia
00:15	04:05	**13:05**	20:05	Fission product yields	D. Brown
00:10	04:20	**13:20**	20:20	Discrete, excited and isomeric states	J-Ch. Sublet
00:10	04:30	**13:30**	20:30	Short break	
00:20	04:40	**13:40**	20:40	Status of proposals	D. Brown
00:20	05:00	**14:00**	21:00	Discussion on next release	All
00:10	05:20	**14:20**	21:20	Version numbers	C. Mattoon, J. Conlin
00:15	05:30	**14:30**	21:30	Review of the GNDS Schema Build System	G. Gert
00:15	05:45	**14:45**	21:45	Discussion on system	All
00:10	06:00	**15:00**	22:00	Requests for format improvements	All
00:20	06:10	**15:10**	22:10	Guidelines for format proposals	All
00:15	06:30	**15:30**	22:30	Mandate extension	D. Brown
	06:45	**15:45**	22:45	Close	

Appendix 3

Revised Mandate

WPEC EXPERT GROUP ON THE RECOMMENDED DEFINITION OF A GENERAL NUCLEAR DATABASE STRUCTURE (EGGNDS)

Members:	All NEA member countries
Full Participant:	European Commission *Under the NEA Statute*
Observer (International Organisation):	International Atomic Energy Agency (IAEA) *By agreement*
Date of creation:	31 May 2016
Start of current mandate:	31 May 2020
Duration:	31 May 2022

Mandate (Document reference):

- Agreed at the 28th meeting of the Working Party on International Nuclear Data Evaluation Cooperation in May 2016 [NEA/SEN/NSC/WPEC(2016)2]
- Approved at the 27th meeting of the NEA Nuclear Science Committee in June 2016 [NEA/SEN/NSC(2016)2]
- Revised and extended at the 30th meeting of the Working Party on International Nuclear Data Evaluation Co-operation [NEA/SEN/NSC/WPEC(2018)2] and endorsed by the 29th NEA Nuclear Science Committee in June 2018 [NEA/SEN/NSC(2018)6]

Context

The Evaluated Nuclear Data File (ENDF-6) nuclear data format has had a long and fruitful history as the preferred format for storing and exchanging evaluated nuclear data. Together with processing codes, it plays a pivotal role connecting nuclear physicists and reactor physicists, allowing them to exchange data between different computer codes. Today, however, it is showing signs of age. In particular, the ENDF-6 format places unnecessary limitations on the types of reactions and the level of precision at which data can be stored, making it more difficult to ensure quality and consistency of the data. Modern users are applying nuclear data towards solving a broad range of problems (in medical physics, global security and advanced detector designs, among others) that stretch the ENDF-6 format beyond its original design.

Purpose, scope and membership

The Subgroup 38 (SG38) of the Working Party on International Nuclear Data Evaluation Cooperation (WPEC) was formed to solicit feedback from international stakeholders and develop a new General Nuclear Database Structure (GNDS) for storing nuclear data to replace the legacy ENDF-6 format. The SG38 has met its stated goal to develop a nuclear data structure definition that can meet the needs of a broad set of nuclear data users and providers.

In order to take the next step, it was necessary to establish an international expert group to endorse, promote and maintain the new format as the future international standard for disseminating nuclear reaction databases. The Expert Group on the Recommended Definition of a General Nuclear Database Structure (EGGNDS) was established in 2016 and became the steward of a new international definition for the modern nuclear database structure.

Goals and activities

The main objectives of this Expert Group are to make the GNDS:

1. easier for new users, as well as current users, to contribute to the community;
2. general and useful enough that it could also be used to organise nuclear structure data, experimental data and other nuclear data products;
3. adhere to high quality assurance and documentation practices.

Other goals include the development of better open source infrastructure to manipulate, search, plot, process, translate and check nuclear data and the development of new nuclear data products heretofore not possible. The EGGNDS will ensure that important and useful tools for using the new recommended definition are developed and maintained.

The EGGNDS will guide the creation of new infrastructure and promote better evaluation practices. It is foreseen that it will release new GNDS versions with appropriate documentation as necessary, without overburdening stakeholders.

Deliverables

The Expert Group will ensure the recommended definition of the GNDS meets the needs of major international nuclear data communities. In addition, this Expert Group will work on the following deliverables:

- release periodic updates of the GNDS specifications that incorporate approved format proposals;
- organise workshops and other outreach activities to train evaluators and other members of the nuclear data community, especially users, on the new structure.