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 Subgroup 43 on Code infrastructure to support a modern general nuclear database (GND) structure

Summary Record

13 May 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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13 May 2020

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SUMMARY RECORD

1. Welcome

The Chair, **F. Malvagi** welcomed the participants (see ***Appendix 1***), including the co-ordindators, **J. Conlin** and **C. Mattoon**, and the WPEC Secretariat, **M. Fleming**.

2. Adoption of the agenda

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

3. EG-GNDS Status Report

D. Brown updated the subgroup on the status of the EG-GNDS following the meeting on 12 May. The GNDS specifications version 1.9, which were approved following the June 2019 meeting, were published as an official OECD report in May 2020. Two complete APIs from LLNL (as discussed below) are on GitHub with partial implementations from ORNL, LANL, CEA and JAEA in the pipeline. Criticality benchmarks are already being run with the GIDI API and these tests will become more extensive and help build the validation case for the new format. Comparing GNDS against the ENDF-6 format, all relevant low-level formats have analogues and a summary of these has been prepared for future publications. The GNDS development version addresses the outstanding issues from the GNDS requirements prepared by SG38, but outstanding issues related to resonance rearrangement, fission product yields and documentation will be dealt with and agreed before the next official release (version 2.0). The work of SG43 is universally recognised as a priority and with the closure of SG43 expected, the EG-GNDS has agreed that the work on championing the adoption of GNDS and co-operation on tools such as APIs can continue within the EG-GNDS mandate.

4. From model code outputs to GNDS -TAGNDS-

J-Ch. Sublet presented work done in a collaboration with **C. Mattoon** to develop GNDS versions of the TENDL evaluations. Initial translation of the ENDF-6 files found that approximately one third of the files could not be translated properly and, since not all data output by the T6 codes can be stored in ENDF-6, there was a strong interest in having a direct method of generating GNDS files. TAGNDS was designed to perform this function

by reading TALYS output data into GNDS classes and serialising these into XML files. The current version is written in Python (2.7 and 3.5 compatible) and requires the development version of FUDGE (not the current version on GitHub.com). Testing has begun with a suite of files and incident particles, with success on all neutron-incident files. Several issues have been identified in this process (e.g. inconsistencies in energy thresholds) and these have been brought to the attention of the developers. At present, the code handles the TALYS outputs but extensions to handle resonances, fission observables and other non-Hauser-Feshbach data are planned, as well as expanded testing.

5. Status of LLNL's GNDS C++ APIs

B. Beck presented the status of the GNDS APIs developed at LLNL, including a suite of five code packages (two C packages, PoPI, GIDI and MCGIDI) that are collectively referred to as GIDI+. The General Interaction Data Interface (GIDI) reads GNDS files and contains classes for GNDS files, which also includes composite and TNSL 'Protare' classes. The PoPI package handles Properties of Particles files while MCGIDI extracts this information and allows sampling for Monte-Carlo codes. Each of these is available within the GIDI+ package that is available at https://github.com/LLNL/gidiplus. The current version only reads the so-called 'GNDS-1.10' LLNL version that is based on the EG-GNDS approved 1.9 version and including primarily the development version updates. The FUDGE code, available at https://github.com/LLNL/fudge is an older version that handles version 1.9 data and should be updated in the near future to also address the LLNL version 1.10 supported by GIDI+.

6. GNDS support in AMPX

D. Wiarda presented the work done at ORNL to handle GNDS formatted data files in a suite of ORNL codes including AMPX, SCALE and SAMMY. This is done through the AMPX in-memory data structures that are used by the other codes. In addition to the low-level access classes, another more convenient layer has been developed which provides more useful utility functions, database access and derived objects. The working plan is for this to be available in one of the upcoming SCALE beta releases and AMPX will be an open source project – although as package within SCALE some logistic issues must be resolved. SAMMY development includes a plan to use this API for resonance evaluations in GNDS format.

7. GNDStk (GNDS Toolkit)

M. Staley presented a new GNDS toolkit (GNDStk) that has been developed by LANL and is available on the NJOY GitHub space https://github.com/njoy/GNDStk. This toolkit allows the reading and writing of GNDS in either XML or JSON, as well as the creation and modification of GNDS trees and conversion between file types. It is written in modern C++ with header-only libraries. Various examples with XML, JSON, node and tree classes were shown. While it is available on GitHub, it is still a work in progress providing low-level, GNDS-specific access.

8. Discussion on SG43 report

C. Mattoon presented the outline of the SG43 report that was been included in a repository in the NEA GitLab at: https://git.oecd-nea.org/science/wpec/sg43/summary-report. The initial outline includes an introduction, description of the goals of APIs and spaces for each of the different code development groups (either complete, in progress or future planned work). In addition to this content on APIs, the numerous physics checking processes will have a space for description, separated by data type. While no GNDS physics checker was developed, the intention in the report is to identify the types of checks that should be made with some reasoning behind the test. The subgroup agreed that the technical details should not be described in this document, which will serve as a summary and will refer to technical publications. The NEA will provide accounts to any participants who require access.

9. Any other business

The participants discussed the continuing need for work that was being done within Subgroup 43. With the GNDS-1.9 specifications published in May 2020, there is a growing interest in GNDS and a need for the APIs and other tools to transition from legacy systems. It was agreed that the work of SG43 in promoting the adoption of GNDS and providing a forum for exchanges on API development should continue and in the immediate future this will occur within the EG-GNDS with a modified mandate of that group. EG-GNDS will also have the responsibility of determining if and when the conditions are right for another fixed-term subgroup within WPEC so that a proposal may be made to the WPEC members.

APPENDIX 1

List of registrants to the 13 May 2020 Meeting of Subgroup 43 on Code infrastructure to support a modern general nuclear database (GND) structure

	Name	Surname	Representing	Notes
1	Bret	BECK	UNITED STATES	
2	David	BROWN	UNITED STATES	
3	Jesse	BROWN	UNITED STATES	
4	Jeremy	CONLIN	UNITED STATES	Co-chair
5	Mark	CORNOCK	UNITED KINGDOM	
6	Michael	FLEMING	NEA	Secretariat
7	Daniela	FOLIGNO	NEA	
8	Tim	GAINES	UNITED KINGDOM	
9	Godfree	GERT	UNITED STATES	
10	Mark	GILBERT	UNITED KINGDOM	
11	Wim	HAECK	UNITED STATES	
12	Michal	HERMAN	UNITED STATES	
13	Andrew	HOLCOMB	UNITED STATES	
14	Raphaelle	ICHOU	FRANCE	
15	Cedric	JOUANNE	FRANCE	
16	Amanda	LEWIS	UNITED STATES	
17	Emily	LEWIS	UNITED KINGDOM	
18	Fausto	MALVAGI	FRANCE	Co-chair
19	Caleb	MATTOON	UNITED STATES	Co-chair
20	Jordan	MCDONNELL	UNITED STATES	
21	Robert	MILLS	UNITED KINGDOM	
22	Benjamin	MURPHY	UNITED STATES	
23	Chris	PERFETTI	UNITED STATES	
24	Danila	ROUBTSOV	CANADA	
25	Allan	SIMPSON	UNITED KINGDOM	
26	Martin	STALEY	UNITED STATES	
27	Jean-Christophe	SUBLET	IAEA	
28	Kenichi	TADA	JAPAN	
29	Ian	THOMPSON	UNITED STATES	
30	Nicholas	THOMPSON	UNITED STATES	
31	Alex	VALENTINE	UNITED KINGDOM	
32	Tim	WARE	UNITED KINGDOM	
33	Dorothea	WIARDA	UNITED STATES	
34	Xiaofei	WU	CHINA	

APPENDIX 2

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

Meeting of Subgroup 43 on Code infrastructure to support a modern general nuclear database (GND) structure

WebEx Meeting

13 May 2020

AGENDA

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:10	06:00	**15:00**	22:00	Welcome	F. Malvagi
00:30	06:10	**15:10**	22:10	EG-GNDS summary	D. Brown
00:20	06:40	**15:40**	22:40	From model code outputs to GNDS - TAGNDS	J-Ch. Sublet
00:30	07:00	**16:00**	23:00	LLNL API report	B. Beck
00:30	07:30	**16:30**	23:30	ORNL API report	D. Wiarda
00:30	08:00	**17:00**	00:00	LANL API report	M. Staley
00:30	08:30	**17:30**	00:30	SG43 summary report	C. Mattoon, J. Conlin
00:15	09:00	**18:00**	01:00	Discussion	F. Malvagi
	09:15	**18:15**	01:15	Close	