Nuclear Energy Agency

NEA/NSC/WPEC/DOC(2019)5

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NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

Working Party on International Nuclear Data Evaluation Co-operation

Meeting of the WPEC Subgroup 45 the Validation of Nuclear Data Libraries (VaNDaL) Project

SUMMARY RECORD

26 June 2019
NEA Headquarters
Boulogne-Billancourt, France

Michael Fleming
+33 1 73 21 28 22
michael.fleming@oecd-nea.org

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
Meeting of Subgroup 45 the Validation of Nuclear Data Libraries (VaNDaL) Project

NEA Headquarters Room BB10
46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

26 June 2019

SUMMARY RECORD

1. Welcome

The Chair, **M. White**, 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 for the meeting.

3. Review of action items and introduction

The Chair, **M. White**, reviewed the original plan of the subgroup 45 activities and the actions from the previous meeting at the ND2019 conference in Beijing. Since the last meeting, **M. Fleming** reviewed the status of the NEA GitLab server. Now that this server is available, participants are encouraged to fulfil the original year one goal and make their contributions to the project available. **M. Fleming** volunteered to assist those groups needing help to complete these actions. **A. Trkov** discussed the suite of inputs he has added from the IAEA NDS validation suite and other participants are preparing materials to be shared. **M. White** discussed issues that will arise as groups try to merge validation suites into jointly managed repositories and encouraged participants to take time this year to consider the licensing issues that may arise. **N. Leclaire** has agreed to lead the effort to draft a QA document for best practices to verify the correctness of benchmark inputs. **W. Haeck** presented progress with JSON formats for sharing validation outputs to be compared and will make the format specification and examples available on the NEA GitLab. He has also volunteered to assist other groups with tools to parse code output into this format.

Most of these initial validation input suites focus on experiments document by the International Criticality Safety Benchmark Evaluation Project (ICSBEP). These documents are maintained by the Working Party on Nuclear Criticality Safety (WPNCS). While there has been considerable attention given to the quality control and revision history of these benchmark specifications, it has been noted that the names for sub-cases within some of the more complex suites of

experiments vary between different suites. This is most evident where the multiple suites describing the same benchmark case have slightly different names. This is a barrier when trying to automate inter-comparison. We continue to seek engagement between WPEC SG45 and the ICSBEP community to rectify this situation and value the wider engagement of NEA staff to help facilitate obtaining closure on this issue.

4. Introduction to the NEA GitLab and SG45 spaces

M. Fleming presented the implementation of the NEA GitLab that occurred in 2018 following the previous WPEC meetings. The WPEC subgroups have spaces within the NEA GitLab that match the organisation of the NEA public website. This includes a subgroup 45 private space that may include multiple git repositories and other subspaces to organise the contributions of the subgroup. As was already noted, this includes a 'contributions' space that already has been populated by the IAEA NDS suite provided by **A. Trkov**. These spaces provide access control mechanisms for those participants who need to maintain tighter controls on their contributions. Anyone requiring these functionalities should consult with **M. Fleming** to see how best to store their contributions.

5. Proposal to adopt C4 for SG45 repositories

M. White presented several observations regarding the control of information and how this is likely to affect the subgroup activities. This is particularly sensitive where multiple groups may wish to share joint development of a validation suite repository. It was noted that while some information is widely shared and made public, such as nuclear structure and reaction data, benchmark information may lie across a line between the public domain and controlled data. It was proposed that the group adopt the Collective Code Construction Contract (C4) [https://rfc.zeromq.org/spec:22] in the development of shared repositories. The participants were asked to consider their needs and restrictions for participating in joint ownership of such a validation suite and be ready to discuss concerns and solutions at the next SG45 meeting.

6. Neutron Balance Data

E. Rozhikhin presented analysis performed to calculate neutron balance data using Russian and American codes, of which many data have been included within the ICSBEP Handbook. This data is of great interest for verifying and understanding the content of the evaluations. Data is provided for all but 252 cases out of 4916 in the 2018 handbook, representing 51 evaluation sets. Known issues that remain include the lack of version control for inputs and balance data, as well as the ability to have only one configuration of each case. More calculations using the continuous-energy ROSFOND cross sections are ongoing. The participants recognised the added value these data bring both to helping verify input deck correctness and their use in validation analysis. It was agreed to include a format for these data within the JSON schema that is in development for cross-comparison.

7. NEA Data Related to SG45 Work

I. Hill reviewed the NEA tools that are of interest for the WPEC subgroup 45 work. This includes the databases behind the ICSBEP and the DICE application that provides access to a wealth of information regarding the benchmarks and data that characterises them. This includes a

XML description of the underlying data within the database which is available on the DVD DICE distributions. Sensitivity profiles, spectra, balance data and other calculated quantities are included with the suite of benchmark data within DICE. It was remarked that for the purpose of cross-comparison, many of these data and the existing XML schema may be used by the group in the development of output data formats.

8. Inter-Comparison Study Results

I. Duhamel reviewed the activities of a cross-comparison study involving LLNL, ORNL and LANL in the US, and IRSN in France. The general idea behind the activity was to compare results from benchmarking calculations between different labs using different codes. Some issues found during the study included the use of different revisions and models for a given case, such as Jezebel, cross-references and use of either the case or evaluation nomenclature for the benchmark, and the exclusion of unaccepted cases in the number series. These are relatively simple to spot in inter-comparisons and help correct errors in cases common to multiple validation suites. Results for 35 HEU cases in the study were shown with ENDF/B-VII.1 calculations and non-negligible differences still under investigation. More systems will be considered in future exercises.

Many of the participants in this effort have developed independent QA procedures for the creation, verification and revision of the input decks use in this process. The relevant documents from each laboratory – WHISPER at LANL, VALID at ORNL and CRYSTAL at IRSN – will be provided through the SG45 GitLab space for the participants to review. N. Leclaire has agreed to lead the effort to draft a QA document that combines the best practices to verify the correctness of benchmark inputs based on the experiences from this work.

9. Input files for VaNDaL and QA

W. Haeck presented an overview of common inputs. He reviewed the different suites available at LANL, including the WHISPER suite that has a QA procedure for criticality safety applications. The general plan for inputs, which represent a component of the subgroup activities, is to consolidate the existing inputs, compare inputs between different codes and prepare a QA document that can be used to create a QA input suite. The primary tests for the inputs will consider nuclide densities, weight fractions and total masses/volumes. Example parsed output data were shown based on a Python parsing tool that has been developed at LANL. The use of this tool can be done by LANL for different files that can be provided to LANL and the outputs can be shared amongst the group until such time as LANL may make the tool(s) open.

10. Proposing a JSON structure for calculation results

W. Haeck presented a proposal for output schema based on the need for cross-comparison studies with multiple participants using different codes. While some quantities, such as k_{eff}, may be simple to compare, it is proposed to include various meta-data including libraries, any options in the simulations, codes and versions, etc. In addition to meta-data, all calculation results should be stored in a rigorously defined schema that ensures all data is captured and can be easily compared. A JSON schema was proposed with basic attributes including types, with several types already defined for preliminary data sharing. Some justifications for choices in the proposed schema were provided and the schema will be made available to subgroup participants to populate with data and/or propose changes. The populated files can be easily parsed and used

for analyses by the participants. A Python interface for the existing JSON schema was shown, demonstrating the ease with which analysis can be performed.

11. Benchmark testing for nuclear data validation at the IAEA

A. Trkov presented the IAEA benchmarking suite and system for performing benchmark studies. This includes more than 2000 cases taken from ICSBEP and SINBAD with an individual input that defines the tested nuclear data libraries. The execution of the testing includes storage of all outputs in a structured manner, with plots and other analyses automatically generated. All nomenclature follows the ICSBEP handbook and DICE system and provides outputs that can be easily parsed by machine. A set of models provided by A. Kahler have been used for 725-group analyses with the IRDFF dosimetry library to address reaction rate data. Results were shown for some series of benchmarks, showing systematic biases with all nuclear data libraries including, for example, the Caliban experiments.

12. Next Meeting and any other business

The next meeting of the WPEC subgroup 45 will be in the week of 11-15 May 2020.

APPENDIX 1

List of participants to the 26 June 2019 Meeting of Subgroup 45 the Validation of Nuclear Data Libraries (VaNDaL) Project

	First Name	Last Name	Country	Notes
1	Hamza	ABBOUDI	MOROCCO	
2	David	BERNARD	FRANCE	*Remote*
3	David	BROWN	UNITED STATES	
4	Yaron	DANON	UNITED STATES	
5	Marie-Anne	DESCALLE	UNITED STATES	
6	Isabelle	DUHAMEL	FRANCE	
7	Michael	FLEMING	NEA	*Secretariat*
8	Zhigang	GE	CHINA	*Remote*
9	Wim	HAECK	UNITED STATES	
10	Ayman	HAWARI	UNITED STATES	
11	Michal	HERMAN	UNITED STATES	
12	Andrew	HOLCOMB	UNITED STATES	
13	Jesse	HOLMES	UNITED STATES	
14	Raphaelle	ICHOU	FRANCE	
15	Osamu	IWAMOTO	JAPAN	
16	Alexis	JINAPHANH	FRANCE	
17	Albert (Skip)	KAHLER	UNITED STATES	
18	Ivan-Alexander	KODELI	SLOVENIA	
19	Luiz Carlos	LEAL	FRANCE	
20	Nicolas	LECLAIRE	FRANCE	
21	Yi-Kang	LEE	FRANCE	
22	Fausto	MALVAGI	FRANCE	
23	Caleb	MATTOON	UNITED STATES	
24	Franco	MICHELSENDIS	NEA	
25	Arjan	PLOMPEN	BELGIUM	
26	Pablo	ROMOJARO	SPAIN	
27	Evgeny	ROZHIKHIN	RUSSIA	
28	Xichao	RUAN	CHINA	*Remote*
29	Stanislav	SIMAKOV	GERMANY	
30	Vladimir	SOBES	UNITED STATES	
31	Alejandro	SONZOGNI	UNITED STATES	
32	Nicolas	SOPPERA	NEA	
33	Jean-Christophe	SUBLET	IAEA	

34	Kenichi	TADA	JAPAN	
35	Andrej	TRKOV	IAEA	
36	Thierry	VISONNEAU	FRANCE	
37	Morgan	WHITE	UNITED STATES	*Chair*
38	Dorothea	WIARDA	UNITED STATES	

APPENDIX 2

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
Meeting of Subgroup 45 the Validation of Nuclear Data Libraries (VaNDaL) Project

NEA Headquarters Room BB10
46 quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, France

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AGENDA

1. Welcome and introductions	Chair
2. Adoption of the agenda	All
3. Review of action items	Chair
4. Introduction to the NEA GitLab and SG45 spaces	M. Fleming
5. Proposal to adopt C4 for SG45 repositories	M. White
6. Neutron Balance Data	E. Rozhikhin
7. NEA Data Related to SG45 Work	I. Hill
8. Inter-Comparison Study Results	I. Duhamel
9. Input files for VaNDaL and QA	W. Haeck
10. Proposing a JSON structure for calculation results	W. Haeck
11. Benchmark testing for nuclear data validation at the IAEA	A. Trkov
12. Next meeting and any other business	

APPENDIX 3

List of actions agreed at the 26 June 2019 Meeting of Subgroup 45 the Validation of Nuclear Data Libraries (VaNDaL) Project

1. **N. Leclaire** to take responsibility for the drafting of a Quality Assurance methods document for input suites
    a. **M. Zerkle** to provide input based on the use of thermal scattering data
    b. **M. White** to provide input based on the experience in forming the WHISPER suite
    c. **V. Sobes / D. Wiarda??** to provide input from the ORNL CS experience in QA of inputs
2. **W. Haeck** to provide the JSON schema for output data to the group through the NEA GitLab
3. **All participants** to provide outputs to LANL for post-processing into JSON format or to generate JSON outputs with the group format
4. **W. Haeck** to generate JSON files for outputs from participants and upload to the shared GitLab space
5. **All participants** to provide inputs within the group GitLab 'contributions' space
    a. **M. White** to provide LANL inputs (conditional upon LAUR process)
    b. **S. van der Marck** to upload NRG suite
    c. **A. Kahler** to upload personal suite
    d. **C. Percher** to provide COG suite of inputs
    e. **P. Romojaro** to provide KENO suite of inputs
    f. **N. Leclaire/IRSN??** to provide MORET inputs
    g. **V. Sobes / D. Wiarda??** to provide ORNL input decks
6. **M. Fleming** to upload DICE nomenclature and revision history file on the subgroup website