

Overview of the OECD-NEA Working Party on International Nuclear Data Evaluation Cooperation (WPEC)

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Abstract. The OECD Nuclear Energy Agency (NEA) Working Party on International Nuclear Data Evaluation Cooperation (WPEC) was established in 1989 to facilitate collaboration in nuclear data activities. Over its thirty year history, different Subgroups have been created to address topics in nearly every aspect of nuclear data, including: experimental measurements, evaluation, validation, model development, quality assurance of databases and the development of software tools.

WPEC has recently completed activities on fission yield evaluation, the general nuclear database structure (GNDS) to replace the ENDF-6 format, methods to provide feedback to evaluation, studies of specific capture cross sections, new methods in thermal scattering kernel evaluation and the Collaborative International Evaluated Library Organisation (CIELO) Pilot Project. Ongoing activities in GNDS application programming interface (API) development, methods for covariance evaluation and quality assurance in nuclear data validation using the International Criticality Safety Benchmark Evaluation Project (ICSBEP) database are complemented by the work of two Expert Groups that oversee the High-Priority Request List (HPRL) for Nuclear Data and the continuous development of the GNDS. New activities on the use of integral experiments for nuclear data validation and adjustment, as well as the use of the Shielding Integral Benchmark Archive and Database (SINBAD) for validation have begun and will be coordinated alongside future Subgroups.

After three decades we will review the status of WPEC, how it integrates other collections and activities organised by the NEA and how it dovetails with the initiatives of the IAEA and other bodies to effectively coordinate international activities in nuclear data.

1 Introduction

Formed in 1989, the Working Party on International Nuclear Data Evaluation Cooperation (WPEC) has brought experts in nuclear data together to co-ordinate activities in experiments, theory, modelling, evaluation and validation. All of the world's nuclear data programmes, including those from NEA member countries, China and the IAEA, pool their expertise to address the largest challenges in their field. WPEC operates by creating 3-year Subgroups that focus on specific scientific topics and advance the

state-of-the-art for that field through a multi-national collaboration. In some cases, WPEC forms long-term Expert Groups to address continually evolving scenarios such as the landscape of priority nuclear data needs. These activities drive improvements in our understanding of the basic physics required to simulate nuclear processes in reactors and other nuclear systems. Multiple major nuclear data libraries have made full or partial releases since the last ND2016 conference that incorporate outputs from virtually every WPEC Subgroup, of which there have been 49 over its 30-year history.

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2 Summary of Current and Recent WPEC Activities

In the following sections we break down the activities of WPEC by topic, describing the progress made and outcomes that have been stimulated by WPEC Subgroups.

2.1 Collaborative International Evaluated Library Organisation Project

Established as WPEC Subgroup 40, The Collaborative International Evaluated Library Organisation (CIELO) Project was an extremely ambitious effort to produce international joint evaluations on the most important (and difficult) isotopes: ^{235}U , ^{238}U , ^{239}Pu , ^{56}Fe , ^{16}O and ^1H . Their evaluation requires the ‘full loop’ of experiments, theory/modelling, evaluation and validation to be considered simultaneously. This Subgroup integrated findings from other WPEC Subgroups and spurred an intense collaboration, involving experts from over 70 institutions, that ultimately delivered as intended [1, 2]. New CIELO evaluations for each of these isotopes have been adopted in the new ENDF/B-VIII.0 [3], JEFF-3.3 [4] and TENDL-2017 [5] libraries. A follow-up activity, focusing on minor plutonium isotopes and some other isotopes has been started at the IAEA as the International Nuclear Data Evaluation Network (INDEN) that operates as a more loosely connected joint project in the spirit of CIELO. A new Subgroup on reproducibility has been established to work hand-in-glove with INDEN and all member country projects by integrating the wealth of NEA-coordinated validation expertise, NEA tools such as NDaST and the new collaborative NEA GitLab platform.

2.2 The High Priority Request List

The OECD-NEA High Priority Request List (HPRL) for Nuclear Data is a reference that stimulates the improvement of nuclear data and bridges the gap between data users and producers. A panel of experts reviews and maintains the list under the WPEC Expert Group on the HPRL. Once approved, requests are classified into high-priority, general or special-purpose requests and entered into a relational database that is publicly searchable on the NEA website. The HPRL entries are annually reviewed and further classified based on the progress that has been made in satisfying the request. New publications on evaluations and experiments are recorded within each entry and used to justify the classification. Numerous new requests have been entered into the HPRL since 2017 and others have been identified as ‘completed’ following the 2018 EG-HPRL review. For a comprehensive review, see [6].

2.3 Generalised Nuclear Data Structures (GNDS)

The current ENDF-6 formats for nuclear data were designed several decades ago, based on legacy computing technology. These formats have not accommodated many new types of information, they store the data very inefficiently and they cause significant waste in computer

programming time to handle legacy technology. They also deter young researchers and engineers who do not want to work with deprecated software paradigms and/or view the community as regressive. A new initiative was started with WPEC Subgroup 38 to design a new structure and format that could be compatible with legacy codes, store data in an extensible and future-proof way and integrate seamlessly with modern programming techniques. The outcomes of this Subgroup included detailed requirements [7, 8] and early draft specification. It was realised that the activity had a great deal of interest from the community and a long-term Expert Group (EG-GNDS) was formed to continue the work, complete a specification document and continually update the specifications over time.

In 2018, the NEA implemented a GitLab system and migrated the EG-GNDS content from the Brookhaven National Laboratory internal servers, giving all participants full access to the working area. This has resulted in a remarkable acceleration and the documentation has nearly doubled in size to a mature state that the group will release as a NEA Publication, with periodic updates for new format extensions. New format proposals and a procedure for approving them have already been agreed, with many new additions expected in the version that follows the GNDS-1.9 release.

To use the new formats, it was realised that a conduit between the data and codes that would use them was required and Subgroup 43 was established to explore this and prepare designs and implementations. In software terminology, this is known as an Application Programming Interface (API) and defines objects that can be used by multiple different programming languages without focusing on the details of the data formats. By designing this API as an international project the mass duplication of effort to perform this for the many nuclear simulation codes around the world would be avoided (as well as the introduction of many errors along the way). Already, multiple APIs have been designed and implemented, including tools such as GIDI [9] and FUDGE [10, 11] that are available with open-source licenses. More are being developed or are planned in the near future.

2.4 Thermal Scattering Kernel $S(\alpha, \beta)$

Thermal scattering of neutrons is an essential part of the physics of neutron interactions in thermalised systems. At these low energies, the physics require different models and data formats than those used in higher energies. This field has been less active since the 1990s, but with new *ab initio* calculation methods and experimental techniques developed in the 2010s, there has been a remarkable resurgence in Thermal Scattering Law (TSL) activity. The WPEC Subgroup 42 was established to bring together experts from around the world to share their methods and data. The result was an unprecedented output, including data for several new materials and phases as well as revisions for essential materials such as light and heavy water. This included a new evaluation for light water ice in response to requests from the criticality safety community. In total,

more new evaluations were made in SG42 than in all countries in the past 30 years. The new releases of ENDF/B-VIII.0 [3] and JEFF-3.3 [4] contain more new evaluations from Subgroup 42 than from any other source. In addition to these new evaluations, new software tools such as *FLASSH* [12] have been developed to overcome approximations within the well-known NJOY LEAPR [13] module and fully utilise new inputs from Density Functional Theory and Molecular Dynamics calculations.

2.5 Resolved Resonance Range Evaluation

Neutron resonance analysis is a specialised topic, relying upon codes developed during the 1970s and manually intensive work that is difficult to reproduce and from which uncertainty information has been difficult to obtain. Two WPEC Subgroups, numbers 36 and 41, primarily led by experimentalists at JRC (EU), JAEA (Japan) and ORNL (USA), modernised models and methods to enable enhanced resonance uncertainty analyses that have been introduced in the most recent evaluations. Subgroup 41 has additionally focused on the evaluation of ^{237}Np and ^{241}Am , combining current measurement work at JPARC/ANNRI (the subject of new EXFOR [14] transmissions in 2019) and evaluation to update capture cross subsections in the resonance range.

2.6 Quality of Input Suites for Nuclear Data Validation

Validation is critical to nuclear data evaluation and performing automatic and Quality Assured (QA) validation is one of the most pressing topics in nuclear data. New initiatives have started under WPEC, as Subgroups 45 (the Validation of Nuclear Data Libraries (VaNDaL) project) and 47, to provide QA inputs for simulation codes and guidance documentation that can be integrated into automatic validation and feedback systems for nuclear data evaluation. Thousands of inputs have been shared from participants for two databases (ICSBEP [15] and SINBAD [16] for Subgroup 45 and 47, respectively) and have been migrated to the NEA GitLab where participants are designing software to compare and QA a set of inputs for various codes. These will ultimately be released to members for use in nuclear data validation and will also be submitted to the Technical Review Groups (TRGs) within the NEA Working Parties on Nuclear Criticality Safety (WP-NCS) and Reactor Systems (WPRS) that oversee these databases. New, extensible output file schema are being defined to perform data mining of the outputs from different simulations, including automatic cross-comparisons between different inputs.

2.7 Integral Feedback and Assimilation

Bringing integral benchmarks into the nuclear data evaluation process has been a focus of the community for many years, as improved computer power and new tools have allowed scientists to ensure that the basic neutron physics comply with integral measurements in a mathematically

rigorous way. Recent advancement in these methods makes them more robust, in terms of physics and support to new evaluations like CIELO, by avoiding compensation effects, providing feedback on nuclear model parameters and prescribing new paradigms in the choice of integral experiments. A large fraction of the High Priority Request List has directly or indirectly benefitted from input from these Subgroups and their predecessor Subgroups, which have included Subgroups 26, 33, 39 and the new Subgroup 46. These methods are expected to have an even greater role in the next generation of nuclear data evaluations, including a new initiative to set revised target accuracies in nuclear applications, translate these requirements through sensitivity analyses into requirements on nuclear data (which is an update from previous WPEC activities [17, 18]) and to prepare adjusted libraries that meet the requirements of a range of advanced reactor technologies.

2.8 Covariance Data in General Purpose Nuclear Data Libraries

New methods for quantifying, storing and propagating uncertainties have been engineered for virtually every area of neutron physics in the past 15 years and methods that are even more sophisticated are in development. The EG-GNDS is developing new formats to store these data, but an interface was required to bring the different communities (thermal scattering, resonances, fission yields, fast energies, etc.) together, establish joint standards and ensure consistency. This was met with WPEC Subgroup 44 on “Covariance Data in General Purpose Nuclear Data Libraries”, which is preparing a reference document that integrates their findings and provides guidance for evaluators in evaluating covariances, alongside a suite of example datasets in existing and new GNDS formats. A pilot study will compare the methodologies and evaluations for cross-correlations between fission cross sections and average fission neutron multiplicities.

2.9 Fission Product Yield Evaluation

WPEC has played a central role in fission product evaluation over decades, with a large number of datasets used by every member country coming directly from WPEC outputs. Several new experimental techniques were developed in the 2010s and, with new simulation and inferential statistics tools available in the past few years, improved fission product yield evaluations and first-of-a-kind correlated uncertainties have become feasible. The most recent Subgroup 37 brought together experimentalists, theoreticians and data scientists to create the first correlated uncertainties and new evaluations that have been used to propagate realistic uncertainties into applications. Outputs from this Subgroup have been directly adopted in new libraries, including the NEA Data Bank organised JEFF-3.3 [19]. This work has helped trigger the IAEA to start a new CRP on fission product yields in 2020 that will be run in parallel to other regional activities.

3 Future WPEC Activities

Following the considerable success with the Subgroup 42 on “Thermal Scattering Kernel $S(\alpha,\beta)$: Measurement, Evaluation and Application,” several recommendations were made: to continue making progress in the development of advanced software that calculates TSL data, to prototype TSL covariances and to continue making new evaluations for more materials. A new Subgroup 48 on “Advances in Thermal Scattering Law Analysis” was established with a mandate based on the Subgroup 42 outcomes.

While the documentation that accompanies the most recent evaluated nuclear data libraries has become much more comprehensive, it remains impractical for most evaluations to be reproduced. This falls short of the goals we have in science, to comprehensively document all work, but also presents a challenge for the nuclear data community to establish QA standards and to manage the considerable knowledge retained by experts not far from retirement. A new Subgroup 49 on “Reproducibility in Nuclear Data Evaluation” was created to capture all of the codes, scripts and data required to create an evaluation. These will be integrated into the NEA GitLab with software containers to prototype a fully reproducible evaluation version control system that can be deployed by the co-operating nuclear data projects in their own library management activities.

More proposals are expected in the 2020 and future meetings. The WPEC welcomes and encourages new contributions and initiatives that further the development of nuclear data evaluations and methodologies. For more information, visit:

www.oecd-nea.org/science/wpec

References

- [1] OECD-NEA, *International Co-operation in Nuclear Data Evaluation: An Extended Summary of the Collaborative International Evaluated Library Organisation (CIELO) Pilot Project*, WPEC Subgroup 40, NEA Publication No. 7498 (2019)
- [2] M. Chadwick et al., Nuclear Data Sheets **148**, 189 (2018), special Issue on Nuclear Reaction Data
- [3] D. Brown et al., Nuclear Data Sheets **148**, 1 (2018), special Issue on Nuclear Reaction Data
- [4] A. Plompen et al., *The Joint Evaluated Fission and Fusion Nuclear Data Library, JEFF-3.3*, in preparation
- [5] A. Koning, D. Rochman, J.C. Sublet, N. Dzysiuk, M. Fleming, S. van der Marck, Nuclear Data Sheets **155**, 1 (2019), special Issue on Nuclear Reaction Data
- [6] E. Dupont et al., *HPRL – International cooperation to identify and monitor priority nuclear data needs for nuclear applications*, ND2019, Beijing, China, 2019
- [7] D. Brown, ed., Tech. Rep. BNL-112394-2016-IR (2016)
- [8] C. Mattoon, B. Beck, N. Patel, N. Summers, G. Hedstrom, D. Brown, Nuclear Data Sheets **113**, 3145 (2012), special Issue on Nuclear Reaction Data
- [9] M.S. McKinley, B.R. Beck, *Implementation of the Generalized Interaction Data Interface (GIDI) in the Mercury Monte Carlo Code, M&C + SNA + MC 2015*, Nashville, TN, United States, Apr 19 – Apr 23, 2015
- [10] B.R. Beck, AIP Conference Proceedings **769**, 503 (2005)
- [11] B.R. Beck, C.M. Mattoon, *FUDGE: A Toolkit for Nuclear Data Management and Processing*, 2014 ANS Annual Meeting, Reno, NV, United States, Jun 15 – Jun 19, 2014
- [12] Y. Zhu, A.I. Hawari, *Full Law Analysis Scattering System Hub (FLASSH)*, PHYSOR 2018, Cancun, Mexico, 2018
- [13] R. Macfarlane, D.W. Muir, R.M. Boicourt, A.C. Kahler, III, J.L. Conlin, Tech. Rep. LA-UR-17-20093 (2017)
- [14] N. Otuka et al., Nuclear Data Sheets **120**, 272 (2014)
- [15] OECD Nuclear Energy Agency, ICSBEP Handbook 2018, DOI:10.1787/ea7c647e-en
- [16] I. Kodeli, A. Milocco, P. Ortego, E. Sartori, Prog. Nucl. Sci. Technol. **4**, 308 (2014)
- [17] OECD-NEA, *International Evaluation Co-operation: Uncertainty and Target Accuracy Assessment for Innovative Systems using Recent Covariance Data Evaluations*, WPEC Subgroup 26, NEA Publication No. 6410, ISBN 978-92-64-99053-1 (2008)
- [18] M. Salvatores et al., Nuclear Data Sheets **118**, 38 (2014)
- [19] R.W. Mills, EPJ Web Conf. **146**, 04008 (2017)