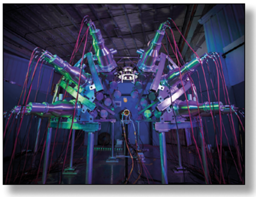
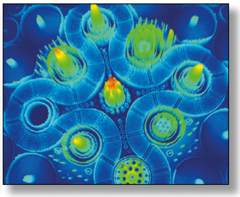
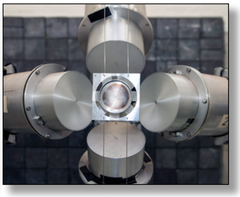
Nuclear Science
2019

International Co-operation in Nuclear Data Evaluation

An Extended Summary of the Collaborative International Evaluated Library Organisation (CIELO) Pilot Project

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NEA No. 7498

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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Cover photos: The Chi-Nu detector array for measuring prompt fission neutron spectra (Los Alamos National Laboratory); Simulation of the Advanced Test Reactor using new CIELO nuclear data files; U-238 sample and detectors for neutron capture measurements (Joint Research Centre, Geel).

Foreword

Complete data representing the relevant nuclear physics are required for the simulation of nuclear systems. These simulations require many types of experimental measurements, theoretical physics, semi-empirical models and software systems, as well as experts to integrate and guide the process. Collectively, the discipline is known as nuclear data. Separate programmes within various European countries, as well as in Japan, Russia, the United States and other Nuclear Energy Agency (NEA) member countries, have been operating such activities for many decades.

The NEA Working Party on International Nuclear Data Evaluation Co-operation (WPEC) was created in 1989, under the aegis of the Nuclear Science Committee (NSC), to improve the quality and completeness of nuclear data by bringing together representatives of the major nuclear data evaluation projects of NEA member countries and of selected invitees. The expert groups and subgroups of the WPEC typically focus on specific technical topics. The Collaborative International Evaluated Library Organisation (CIELO) Pilot Project, working under the auspices of the WPEC Subgroup 40, was established to generate complete evaluations for a selection of the most important isotopes for parameters in nuclear technologies: ^{235}U, ^{238}U, ^{239}Pu, ^{56}Fe, ^{16}O and ^{1}H with the aim of improving the accuracy of the data and resolving previous discrepancies in the overall understanding

The CIELO Pilot Project has been overseeing numerous activities, which recently resulted in an entire special issue of the *Nuclear Data Sheets* journal (Issue 148, 2018) being dedicated to the subject. It has also led to the production of a suite of new nuclear data evaluations that have been incorporated into major nuclear data libraries. The outcomes of evaluations include significant harmonisation of discrepancies between independent programmes, improvements in the performance of international standard nuclear criticality and neutron transmission benchmarks, complete uncertainties for nearly all parameters and the use of modern data storage technologies. Overall, this work has leveraged considerable, parallel and experimental work in collecting improved experimental measurements to support nuclear data, while highlighting high-priority areas for further study. A productive and durable framework for international evaluation was thus established to build upon lessons learnt. These lessons will continue through new WPEC groups and a new International Atomic Energy Agency (IAEA) evaluation network, which was initiated in response to the success of the NEA CIELO Pilot Project.

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List of abbreviations and acronyms

AMS	Accelerator mass spectrometry
ATLF	Above-thermal leakage fraction
BNL	Brookhaven National Laboratory (United States)
BROND	Russian Evaluated Neutron Data Library
CAB	Centro Atómico Bariloche (Argentina)
CEA	Commissariat à l'énergie atomique et aux énergies alternatives (France)
CENDL	China Evaluated Nuclear Data Library
CERN	European Organization for Nuclear Research
CERN n_TOF	Neutron time-of-flight facility at CERN (France)
CIAE	China Institute of Atomic Energy
ENDF	Evaluated Nuclear Data File
CIELO	Collaborative International Evaluated Library Organisation (NEA pilot project)
CIELO-1	Sets of CIELO cross section data adopted by the ENDF community
CIELO-2	Sets of CIELO cross section data adopted by the JEFF community
DANCE	Detector for Advanced Neutron Capture Experiments
DDCOM	Dispersive coupled-channel optical model
FCA	Fast critical assembly
FWHM	Full width at half maximum
GELINA	Geel Electron LINear Accelerator Facility (Belgium)
HEU	Highly enriched uranium
HMF	Highly enriched uranium metal with fast neutrons
HST	Highly enriched uranium solutions with thermal neutrons
IAEA	International Atomic Energy Agency

ICSBEP	International Criticality Safety Benchmark Evaluation Project (NEA)
IPPE	Institute of Physics and Power Engineering (Russia)
IRSN	Institut de Radioprotection et de Sûreté Nucléaire (France)
JAEA	Japan Atomic Energy Agency
JEFF	Joint Evaluated Fission and Fusion File (NEA)
JENDL	Japanese Evaluated Nuclear Data Library
JRC	Joint Research Centre (European Commission)
LANL	Los Alamos National Laboratory (United States)
LCT	Low-enriched uranium compound with thermal neutrons
MCNP	Monte Carlo N-Particle Transport Code
NDaST	Nuclear Data Sensitivity Tool (NEA)
NRG	Nuclear Research and Consultancy Group (Netherlands)
NSC	Nuclear Science Committee (NEA)
Nubar	Average number of neutrons per fission
NUEX	Neutrino excitation of nuclear levels
ORELA	Oak Ridge Electron Linear Accelerator (United States)
ORNL	Oak Ridge National Laboratory (United States)
PFNS	Prompt fission neutron spectra
PMF	Plutonium metal with fast neutrons
PST	Plutonium thermal solutions
ROSFOND	Russian National Library of Neutron Data
RPI	Rensselaer Polytechnic Institute (United States)
TSL	Thermal scattering law
TUNL	Triangle Universities Nuclear Lab (United States)
WPEC	Working Party on International Nuclear Data Evaluation Co-operation (NEA)
ZPR	Zero Power Reactor

Motivation for the work

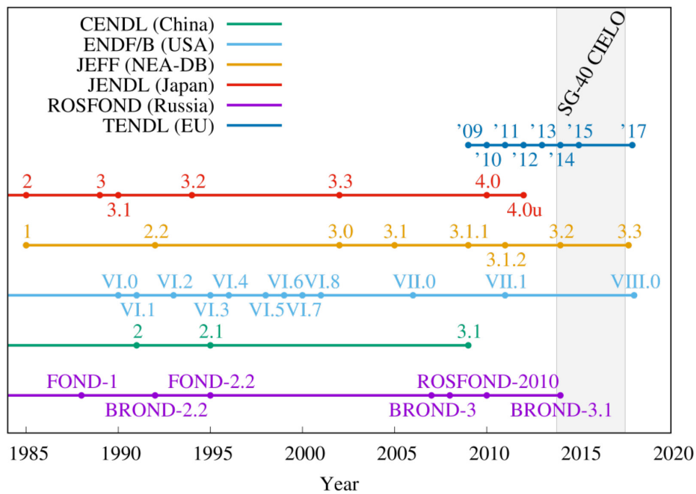
The physics of nuclear reactions embodies essential information for the design, operation and decommissioning of nuclear systems, with applications spanning energy, safety, medicine, science, security and a great many other industrial processes. The types of knowledge required are as diverse as the applications, including on reaction probabilities (cross-sections) for many different types of reactions, emitted particle probabilities/energies/angles, probabilities for different fission fragment formation, and decay processes and their emitted particle data. Many of these data vary with the incident particle energy, potentially by factors of one million or more. In addition to the above requirements, it is important to have correlated uncertainties for all data in order to quantify and propagate uncertainties in simulations.

A general-purpose nuclear data library must therefore contain all of this information. It is the role of the nuclear data evaluators to craft databases of information for all of the elements and isotopes that may be required. Through the Nuclear Energy Agency (NEA) international EXFOR database, evaluators have access to a wealth of experimental data to guide this process, but only a small fraction of a library can be directly compared with measurements as a result of the extensive requirements for a general purpose library. Models and computer codes are developed not only to fill these gaps, but to ensure consistency of the data. Because of the fundamental challenges presented by the different aspects of relevant nuclear physics, there is no single model or code that can calculate more than a fraction of the required data. As a result, many models are in use within every major nuclear data programme, of which there are several that currently exist around the world. The integration of these many systems and their respective communities of experts is the main challenge that nuclear data programme managers face in organising the delivery of improved nuclear data files.

Each of the major, general purpose nuclear data projects, including ENDF (United States), JEFF (NEA Data Bank), JENDL (Japan), CENDL (China) and ROSFOND (Russia), develop and release libraries that include numerous isotopes. An overview of the progress and history of the libraries released is shown in Figure 1 below.

The libraries draw largely on each other, implicitly recognising the qualities of the other projects and their data files. Taking files for five americium isotopes of the most recent JEFF-3.3 as an example; one (^{241}Am) is an evaluation resulting from the JEFF community, while two (^{244}Am and ^{244m}Am) are taken from the JENDL Actinoid File 2008 and two (^{242}Am and ^{242m}Am) are from a 1996 Belarusian evaluation (Maslov, et al. 1997) that was incorporated into the JENDL-3.3 library. A more detailed inspection of these files reveals that they are also the product of multiple projects. For example, several of the major curium isotopes, including ^{242,244,245}Cm, include original work from the JEFF community, as well as fission photon multiplicities and distributions from ENDF/B-VII.1, fission angular distributions for particles from BROND-2.2, and resonance parameters and fission neutron covariances from JENDL-4.0. These *mélanges* do not represent a problem, but rather they demonstrate the regard that evaluators have for the work of their counterparts around the world.

Figure 1. Overview of the well-known nuclear data libraries and their releases



The routine adoption of data or of complete files between different nuclear data projects underlines an essential fact: that major nuclear data projects have been collaborating for several decades. This indirect collaboration has not benefited from the co-operation and co-ordination that occurs within each project. The Collaborative International Evaluated Library Organisation (CIELO) Project was proposed to facilitate this missing, direct and natural collaboration for a set of high-priority isotopes.

While the objective of the CIELO Project was to discuss, understand and document discrepancies, it was not necessarily to resolve all of these discrepancies. It must be recognised that each evaluation may prioritise different experimental data or models, target different applications, or elect to use different mechanisms to reach a final file (e.g. use of integral adjustment). Despite official CIELO files being produced as a result of the subgroup activities (referred to below as the CIELO-1 and CIELO-2 files), not one set was agreed upon by all participants. This result is by itself an important development. In fact, one important CIELO outcome was an appreciation for the fact that there must be room for differing ideas in any scientific endeavour.

New experimental measurements

The data within nuclear data libraries cannot be derived from first principles, and experimental measurements form the basis of all evaluations. These represent significant costs, in terms of funding, time and the availability of suitably trained (and talented) experimental physicists. Requests for more accurate measurements require the development of new concepts and equipment, which in turn require more resources.

Motivated by the new evaluation efforts in the Collaborative International Evaluated Library Organisation (CIELO) Pilot Project, several new measurement campaigns were performed in the United States and Europe. Table 1 summarises the contributions made since 2013, available for use in the production of the CIELO files, which form the primary deliverable of this subgroup. For more details on the experiments and their use in the CIELO evaluation process, see the main reference paper (Chadwick, et al. 2018) and others within that *Nuclear Data Sheets* 148 special issue. It should be noted that these do not include the recent measurements that were taken into account in the creation of the new International Atomic Energy Agency (IAEA) standards (Carlson, et al. 2018) and that are documented in this report.

Table 1. Notable experimental contributions during the course of the CIELO project since 2013

Laboratory	Measured data for CIELO
CERN n_TOF	$^{235,238}U$ fission cross sections $^{235,238}U$ neutron capture cross sections
JRC-Geel	^{238}U neutron capture cross section Fe inelastic scattering cross section $^{16}O(n, \alpha)$ cross section
LANL	$^{235,238}U$, ^{239}Pu fission cross sections $^{235,238}U$, ^{239}Pu neutron capture cross sections Prompt fission neutron spectra Iron inelastic gamma production
RPI	^{235}U fission cross section ^{235}U, Fe neutron capture cross sections ^{238}U and Fe semi-differential scattering ^{16}O total cross section
TUNL	$^{238}U(n,2n)$ cross sections

CIELO evaluated files

The Collaborative International Evaluated Library Organisation (CIELO) Project focused on six isotopes, including the "big three" actinides, ^{235}U, ^{238}U and ^{239}Pu, as well as the primary structural material, ^{56}Fe, and two isotopes that are present in numerous materials, ranging from ceramics and oxides to organic matter and water: ^{1}H and ^{16}O. While these have been the subject of many experiments and nuclear data evaluations, and are the primary components of systems that have been built with input depending upon validated nuclear data libraries, differences among data in major evaluations are still common and often greater than the evaluated uncertainties. By bringing together experts from multiple evaluation projects, and with the benefit of the most recent and accurate experimental data, new evaluated files have been created.

In the creation of new evaluations, it is essential to study the full breadth of relevant physics, including fission, average neutron emission and energy spectra, scattering, and capture. Only by considering all of these simultaneously, for all isotopes, has progress been made on building upon the performance of previous evaluations and improving the performance on targeted benchmarks. The following sections provide some description of the important findings of this work.

Fission in ^{235}U and ^{239}Pu

Recent IAEA standards (Carlson, et al. 2018) have been issued, which have doubled the uncertainties on fission cross sections as a result of large (1.2%), systematic uncertainties that were unrecognised in previous experiments. Efforts were made to ensure compatibility with both these new standards and the uncertainties in the CIELO files for ^{235}U and ^{239}Pu. The uncertainties translate directly into increased uncertainties when calculating quantities such as k_{eff} criticality, and they have a significant impact on many analyses, including statistical comparisons with benchmarks when nuclear data uncertainties are considered (Capote, et al. 2018). Although these new fission cross-section uncertainties represent an increase compared to earlier assessments, the standard subject matter experts view them as more credible. Furthermore, future experimental work might lead to reduced uncertainties.

The prompt fission neutron spectra (PFNS) provide the source neutron spectra in a critical fission system, and new experimental evidence has supported a distribution with a greater lower-energy component, or "softer" spectrum, for both thermal fission and fission for ~MeV-range incident neutrons on ^{235}U. These findings have been incorporated into new PFNS evaluations for ^{235}U (Neudecker, et al. 2018). The experiments for ^{239}Pu are ongoing, and it is expected that future work will be able to revisit the plutonium PFNS.

The average total neutron yield per fission, or *nubar*, is a highly sensitive quantity for criticality calculations, and it is routinely adjusted within the experimental uncertainties by evaluators in order to optimise agreement with integral experiments. This is unlikely to change in the foreseeable future as the current experimental methods appear to have reached limits that will be difficult to improve upon.

Capture and scattering in $^{235,238}U$ and ^{239}Pu

Moving beyond the fission-related quantities in actinides, the ratios with capture cross sections dictate the fractions of neutrons that undergo fission rather than being absorbed. These have benefited from several capture ^{238}U measurements that have been used in the *IAEA Neutron Standards* (2006 and 2017), which have been integrated within CIELO. Experimental evidence has also motivated the decrease of the ^{235}U capture cross section from ENDF/B-VII.1 near 1 keV and an increase in the 10 keV region. Future experiments will be useful to corroborate these changed assessments.

Neutron scattering plays a central role in neutron transport and in reducing energy and controlling the flight paths of neutrons in a system. New, semi-differential measurements from the Rensselaer Polytechnic Institute and theoretical models have resulted in new ^{238}U inelastic scattering evaluations, and future measurements are planned for ^{239}Pu. Likewise, uncertainties in the ^{235}U scattering cross sections in the fast energy range, 100s of keV to MeVs, will require new measurements similar to those performed for ^{238}U.

The evaluations in CIELO for these isotopes benefitted greatly or directly adopted data that was produced in another WPEC activity under Subgroup 34 (NEA, 2014).

Evaluation of ^{56}Fe

The evaluation of iron requires a very detailed representation of the resonating cross sections up to a relatively high energy in the MeVs. Coupled with the requirement to adequately account for the capture and scattering processes, it presents a challenge that the available experimental measurements do not adequately constrain. As a result, the space of justifiable evaluations is quite broad, and the evaluator has a great deal of flexibility in selecting the final data. The consequence of this flexibility is that adjustments to iron are made to optimise results for integral criticality and transport benchmarks, which must be undertaken in concert with the other isotopes to which the benchmarks are sensitive. Since these are, for most benchmarks, the very isotopes considered in the CIELO project, the performance for the CIELO-1 and CIELO-2 based libraries, ENDF/B-VIII.0 and JEFF-3.3, are quite good (Herman, et al. 2018). Further experimental data that could better constrain these evaluation parameters would greatly simplify this process and assist in harmonising international nuclear data evaluations. It has also been noted that future work on the elastic and inelastic scatter cross sections, as well as their angular distributions, is required in order to improve the simulation of neutron transmission through macroscopic quantities of iron.

Evaluation of ^{16}O

The participants were able to reach a consensus on the values for the low-energy neutron elastic scattering cross section and the magnitude of the total cross section up to the fast energy range. The coupling of R-matrix analyses with rigorous studies of the available experimental data assisted in this, as well as in the evaluation of the (n,α) cross section. Nevertheless, different assessments of the $^{16}O(n,\alpha)$ cross sections were made in the CIELO-1 and CIELO-2 libraries – future accurate experiments would be valuable to resolve these discrepancies. In contrast, the ^{1}H evaluations were jointly adopted in both CIELO-1 and CIELO-2.

Final CIELO file versions

While harmonisation of evaluations was a stated goal of the CIELO project, the objective was not to generate one monolithic evaluation.

> As the uncertainty data (available in nearly all components of the CIELO files) indicate, it is not possible to make one authoritative evaluation that reflects the experimental measurements, let alone nature. It is worth considering that "[the] alternative to uncertainty is authority, against which science has fought for centuries" (Gleick 1993).

To accommodate the two, self-consistent evaluated file sets that emerged from the CIELO activities, two versions were issued. These were labelled CIELO-1 and CIELO-2 and were later adopted by the ENDF/B-VIII.0 and JEFF-3.3 libraries, respectively. The contents of these evaluations are numerous but can be generally broken down into one component for the resonance energy (where cross sections vary by orders of magnitude) and the fast energy ranges. These are typically evaluated separately and integrated to create the final file. Table 2 summarises the leading laboratory or group that evaluated these components for each file in both of the CIELO versions. It should be noted that these versions do not represent two evaluations from two segregated communities. Files from the US Oak Ridge and Los Alamos National Laboratories appear in CIELO-2 and files from the EU Joint Research Centre Geel and the French Alternative Energies and Atomic Energy Commission (CEA) appear in CIELO-1. Indeed, some results from participants in the JEFF community were selected for CIELO-1 and not for CIELO-2.

Table 2. Lead laboratories evaluating CIELO-1 and CIELO-2 databases

Isotope	CIELO-1	CIELO-2
^{1}H	LANL/IAEA	LANL/IAEA
^{16}O res.	LANL/JRC-Geel	IRSN/JRC-Geel
^{16}O fast	LANL	LANL
^{56}Fe res.	IAEA/BNL	IRSN
^{56}Fe fast	BNL/IAEA/CIAE	JEFF
^{235}U res.	ORNL/IAEA	IRSN/ORNL
^{235}U fast	IAEA+LANL PFNS	CEA
^{238}U res.	JRC-Geel	IRSN/CEA
^{238}U fast	IAEA+LANL PFNS	CEA
^{239}Pu res.	ORNL/CEA	ORNL/CEA
^{239}Pu fast	LANL	CEA

Integral benchmarking

Experimental data, such as those provided by the new measurement campaigns listed in Table 1, are essential for determining the detailed, energy-dependent values in evaluated files. However, they do not account for information on the behaviour of full systems of interest to the users of nuclear data. In order to test – and often to improve – the physics in the nuclear data libraries, full simulations of macroscopic systems are used. These are referred to as "integral" experiments, since they effectively integrate the various reaction rates and physics over a range of energies. If agreement is found for some integral measurement, it helps validate the data for the system considered. By validating a suite of nuclear data files for a large number of independent benchmarks, confidence can be developed in the results of simulations for systems that are similar to those within the benchmarking suite.

The standard metric for testing nuclear data libraries is the "reduced" chi-squared:

$$\chi^2 = \frac{1}{k}\sum_i^n \frac{({}^{C_i}/_{E_i} - \mu)^2}{{\sigma_i}^2},$$

where the calculated and experimental values C_i and E_i are compared with the averaged value μ, mediated by the uncertainty σ_i. The degrees of freedom, k, are considered in these analyses to be equal to the number of experiments considered and the experimental uncertainties alone are considered. There are many complexities raised by the possibilities of considering nuclear data uncertainties and correlations between the benchmark measurements, but these are beyond the scope of the current report.

Reduced chi-squared can be used to test whether the calculated values for a set of benchmarks are different from the experimentally measured values in a statistically significant way. *No single value is necessarily better or worse than another*, but larger values are generally *less likely*. It must be stressed that if all the experimental uncertainties were accurate, and all the calculated values reflected the true physics perfectly, the chi-squared value would *not be zero*. The expectation value, which many consider a target value, would be approximately one.

The use of criticality and neutron transmission experiments, available within NEA benchmark collections,[1] was part of an iterative process in the CIELO work, with feedback from results and sensitivity analyses providing guidance for evaluators to focus their efforts. The NEA Nuclear Data Sensitivity Tool (NDaST; Dyrda, et al. 2017) was used to analyse sensitivity profiles of thousands of benchmarks and pinpoint specific reactions and energies where updates would improve the evaluated files. There remains an ongoing concern that the use of integral feedback undermines the exercise of validating nuclear data, as the files could be tailored to simply reproduce those results. However, to ensure the highest-quality evaluations, experts use all available information to model the physics in a way that is faithful to the theory and available, differential measurements. The criticism also does not account for the fact that the tailoring, or "tuning" of a data file, is typically done to match a small fraction of the available integral data, and the improved databases are then compared against very large compilations of other integral data.

Results presented here were obtained by processing the evaluated nuclear data files with the NJOY code (MacFarlane, et al. 2018) and then simulating a set of benchmark scenarios using the MCNP® version 6 Monte Carlo transport code (Goorley, et al. 2012).

Results with the Mosteller suite

Although there are thousands of benchmarks that were considered in the Collaborative International Evaluated Library Organisation (CIELO) Pilot Project, a subset of 119, known as the "Mosteller suite" have been systematically modelled in MCNP® by the Los Alamos National Laboratory, which is responsible for the code itself. Final results for the CIELO-1 and CIELO-2 evaluations, as well as the ENDF/B-VII.1 results, for reference, are shown in Figure 1 alongside the values for CIELO-1 (as adopted in ENDF/B-VIII.0) and CIELO-2 (as adopted in JEFF-3.3). The improvement seen for ENDF is similar for the JEFF library with the new version. A small subset of these benchmarks is responsible for the majority of the total chi-squared value. Most notably, those of the Jemimas (fast spectrum, metal with intermediate-enriched uranium) and ZEUS (intermediate spectrum, metal with highly enriched uranium) benchmarks provide nearly half of the chi-squared for ENDF/B-VII.1. This represents cases with differences between the calculated and experimental criticality values that are many multiples of the experimental uncertainty. The new CIELO evaluations reduce these by better than half, dominating the improvement in performance as represented by a decrease in the total chi-squared.

While the CIELO-1 chi-squared value is slightly lower than that for CIELO-2, it should be noted that these are still largely a result of a small subset of benchmarks. For example, the difference between CIELO-1 and CIELO-2 for Jemima-4, Thor and two of the ZEUS benchmarks are each, individually, greater than the difference in the

1 The NEA benchmark collections include neutronic parameters other than criticality (e.g. flux distributions, spectral indices, reactivity data, β_{eff} and others).

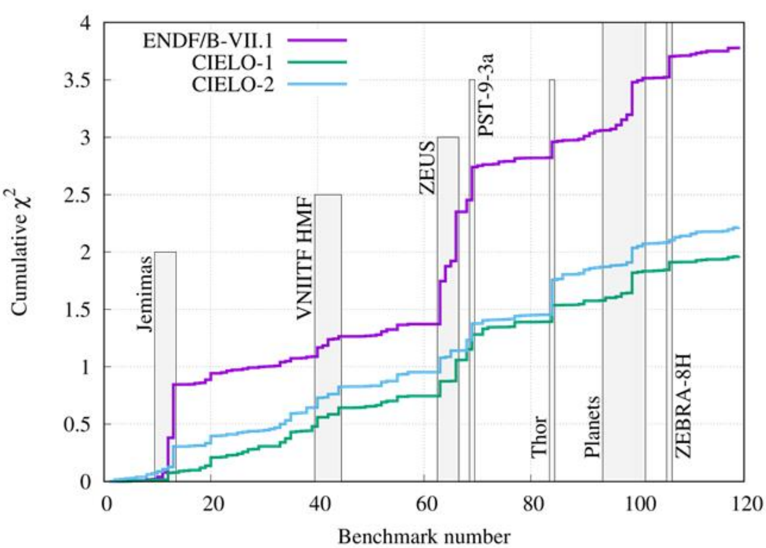
total chi-squared between these two evaluations. If the performance on just one of these was reversed, the apparent superiority between these two would be reversed. This underlines the sensitivity of this statistic on individual cases, as well as the fickle nature of chi-squared comparisons and the selection of benchmark cases. However, the better agreement found for all these challenging benchmarks, while retaining excellent performance in all other cases, is a significant accomplishment.

Breaking down the results by benchmark materials, as seen in Figure 2, offers a perspective on the systems that have been affected by the new data files. These are classified as systems made of:

- PU for plutonium;
- HEU for highly enriched uranium;
- IEU for intermediate-enriched uranium;
- LEU for low-enriched uranium;
- ^{233}U for systems with the ^{233}U isotope (rather than $^{235,238}U$);
- MIX for plutonium-uranium mixtures.

It should be noted that these include cases ranging from bare metal sphere to solutions, with a range of geometries and average neutron spectra, as well as experiments from several NEA member countries.

Figure 1. Cumulative, reduced chi-squared values for the Mosteller suite of criticality benchmarks



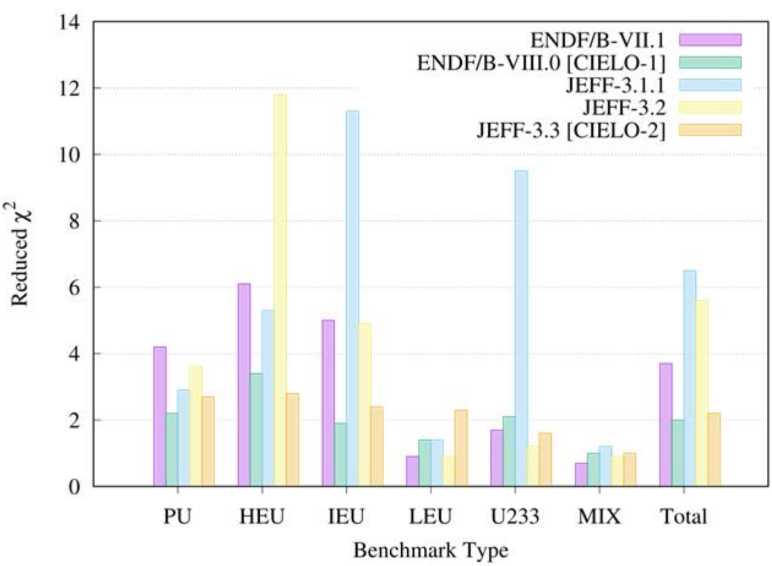
Note: CIELO-1 (as ENDF/B-VIII.0) and CIELO-2 (as JEFF-3.3) results are compared with those of ENDF/B-VII.1. A selection of benchmarks with noteworthy results is highlighted.

Source: Adapted from *Nuclear Data Sheets* 148, February 2018: 189-213.

The general result for both ENDF and JEFF is a decrease in the total chi-squared values for several systems that have large values with previous releases. CIELO-1 is responsible for improving the ENDF/B-VIII.0 plutonium, highly- and intermediate-enriched ^{235}U uranium benchmarks. The CIELO-2 impact on the JEFF files is similarly impressive, with considerable improvement for the highly- and intermediate-enriched uranium. The low-enriched subset is more difficult to reconcile and may require further study for CIELO-2.

The fluctuations between the different JEFF releases in the highly enriched benchmarks highlight a very important feature that may be forgotten by readers who are accustomed to seeing figures of universal improvement: it is very challenging to produce nuclear data evaluations that correct some discrepancy with experiment, while maintaining the same performance in all other benchmarks.

Figure 2. Breakdown of the 119 "Mosteller suite" reduced chi-squared results by material, considering previous and current releases of the ENDF and JEFF libraries, which now contain the CIELO-1 and CIELO-2 evaluated files



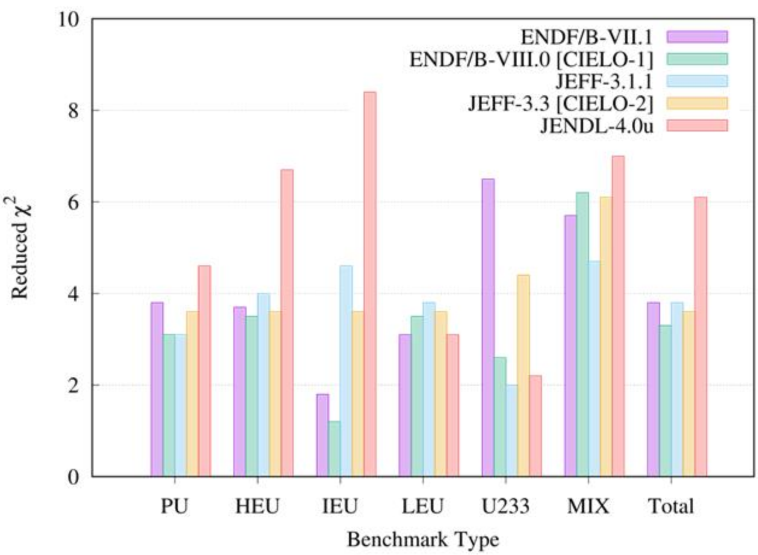
Source: Adapted from *Nuclear Data Sheets* 148, February 2018: 189-213.

Results with the van der Marck suite

While the Mosteller suite of 119 benchmarks is highly regarded for the purpose of integral testing, there are thousands of integral measurements within the International Criticality Safety Benchmark Evaluation Project (ICSBEP). The ICSBEP is not specifically tasked with the production of input files for simulation codes, and such suites of files require significant efforts to produce. The set of MCNP® inputs created by S. van der Marck, of the Dutch Nuclear Research and Consultancy Group, includes 1766 cases. Reduced chi-squared results for the breakdown of benchmarks by material are shown in Figure 3.

Over this large set of benchmarks, the trends are more difficult to interpret. The ^{233}U evaluation in ENDF/B-VIII.0 is a new file, based on JENDL-4.0 with updates to the 2006 *IAEA Standard* and with an increase to the average neutron release in the epithermal energy range. These substantially decreased the chi-squared values in several benchmarks. The JEFF-3.3 ^{233}U file is taken from ENDF/B-VII.1 and is responsible for the increase in chi-squared. It must be stressed that these values are dominated, as in the Mosteller suite shown in Figure 1, by a subset of benchmarks with discrepant results. Clearly, not all of these were targeted in the CIELO project and the significant improvement in the Mosteller suite does not translate directly to a comparable improvement in some other sets of benchmarks.

Figure 3. Breakdown of the 1766 "van der Marck suite" reduced chi-squared results by material, considering previous and current releases of the ENDF and JEFF libraries, which now contain the CIELO-1 and CIELO-2 evaluated files, as well as the JENDL-4.0u library



Source: Adapted from *Nuclear Data Sheets* 148, February 2018: 189-213.

Uncertainty analyses on criticality benchmarks

Uncertainty calculations have been performed using the NEA NDaST tool, which couples benchmark sensitivity matrices with input nuclear data covariances. Examples of the uncertainties in the nuclear data at 1 MeV were shown in Tables 6 and 7 in the *Nuclear Data Sheets* paper by Chadwick (2018). The results for the Jezebel fast plutonium sphere assembly are shown in Tables 3 and 4, and results for the fast Godiva highly enriched uranium sphere assembly are shown in Table 6. The values shown in this table illustrate some of the points emphasised earlier in this report on covariances, namely:

- the k_{eff} uncertainties calculated from the covariances largely exceed the measured uncertainty (second row from bottom), yet the mean values agree very well (bottom row), reflecting the calibration process that was employed;
- there are significant differences sometimes in uncertainties from individual reaction channels that our subject matter experts assess;
- uncertainties do not always diminish with time; sometimes the new evaluations embody larger uncertainty assessments, reflecting a view that the previous assessments were unrealistically small, and that previously-unappreciated systematic errors have been identified.

The Jezebel plutonium benchmark demonstrates the effects of the new fission cross section uncertainties introduced via the *IAEA Neutron Standards*, as well as an increase in the PFNS uncertainties. It must be noted that anti-correlations between reaction channels decreases the summed uncertainty below what would be expected from a fully uncorrelated case. The Godiva benchmark shows a more complex picture for the change between ENDF/B-VII.1 and the CIELO-1 based ENDF/B-VIII.0, where fission and capture channels have substantially changed their covariances, resulting in, respectively, increases and decreases that are nearly equivalent. The decrease in the PFNS uncertainty because of the new evaluation and new inelastic covariance data results ultimately in a lower uncertainty. For the Godiva benchmark, this uncertainty (1 036 pcm) is, as expected, well above the experimental value of 100 pcm. This reflects a well-known fact that some integral experiments are more precisely measured than individual, fundamental quantities (e.g. a specific cross section or emitted energy spectrum) to which the integral values are sensitive.

> The large spread in values between uncertainties in the major nuclear data libraries highlights the fact that this is an active area of research with significant, ongoing revision much greater than the evaluation of the nominal data. Understanding the methodologies behind these evaluations will be a major focus for upcoming activities.

The values quoted in Tables 3 and 4 are not in entire agreement with those of the CIELO *Nuclear Data Sheets* publication, as a result of the adjustment of covariance matrices that occurred between the fifth and sixth release candidates of CIELO-1. Between these two versions, inelastic scattering cross section and *nubar* covariances were re-evaluated, ultimately reducing k_{eff} criticality uncertainties, in the case of the Godiva benchmark, by over 400 and 100 pcm, respectively. The values in this report reflect the final ENDF/B-VIII.0 and CIELO-1 evaluations.

Table 3. Uncertainties for the Jezebel (PMF1) benchmark criticality (k_{eff}), based on NDaST and MCNP simulations that use the ^{239}Pu covariance uncertainty data as calculated

	ENDF/B-VIII.0 Jezebel k_{eff} Unc.	ENDF/B-VII.1 Jezebel k_{eff} Unc.	JEFF-3.3 Jezebel k_{eff} Unc.	JENDL-4.0u1 Jezebel k_{eff} Unc.
	(pcm)	(pcm)	(pcm)	(pcm)
Fission	903	331	305	434
ν (nubar)	316	81	413	209
PFNS	188	186	443	286
Elastic	462	438	90	198
Inelastic	785	797	150	250
Capture	66	74	30	59
Correlated Sum	**±1 041**	**±562**	**±645**	**±648**
Exp. Uncert.	±110			

Notes: Units are in pcm, which is 1 in 100 000 of keff. The summed value is less than the summed individual values in quadrature owing to correlations between the various channels. The experimental uncertainty on k_{eff} is shown for comparison, where here we show the most recent PMF1rev4 assessment as opposed to the older uncertainty value of 200 pcm. All uncertainties are quoted at the 1-sigma confidence level.

Table 4. Uncertainties for the Godiva (HMF1-1) benchmark criticality (k_{eff}), based on NDaST and MCNP simulations that use the ^{235}U covariance uncertainty data

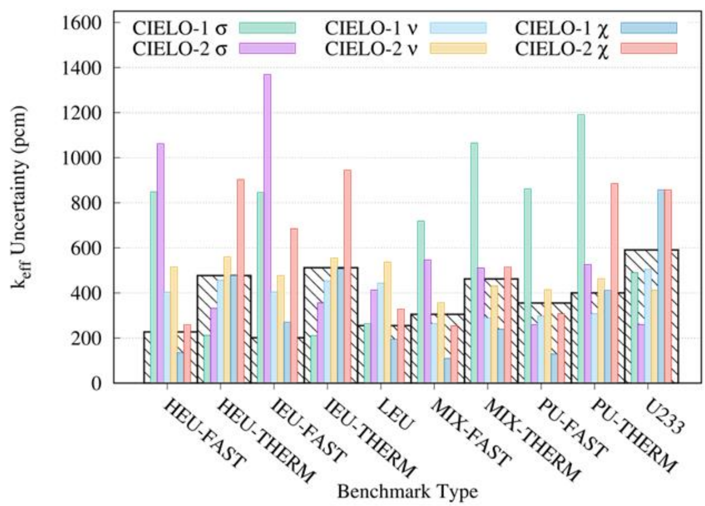
	ENDF/B-VIII.0 Godiva (HMF1-1) k_{eff} Unc.	ENDF/B-VII.1 Godiva (HMF1-1) k_{eff} Unc.	JEFF-3.3 Godiva (HMF1-1) k_{eff} Unc.	JENDL-4.0u1 Godiva (HMF1-1) k_{eff} Unc.
	(pcm)	(pcm)	(pcm)	(pcm)
Fission	788	269	648	320
ν (nubar)	400	545	510	274
PFNS	124	276	364	176
Elastic	276	294	109	426
Inelastic	244	616	698	681
Capture	281	873	375	269
Correlated Sum	**±1 036**	**±1 220**	**±1 342**	**±962**
Exp. Uncert.	±100			

Notes: Units are in pcm, which is 1 in 100 000 of keff. The summed value is less than the summed individual values in quadrature owing to correlations between the various channels. The experimental uncertainty on k_{eff} is shown for comparison. All uncertainties are quoted at the 1-sigma confidence level.

The global picture of uncertainties may be probed using the NEA NDaST tool, as shown in Figure 4. Both the CIELO-1 and CIELO-2 evaluated covariances have been analysed, with uncertainties broken down into:

- [σ] the correlated contributions from all cross-section uncertainties, including both energy-dependent correlations for each reaction channel *and* correlations between different reaction channels, as one cross section uncertainty;
- [ν] the uncertainties from the neutron yield per fission, or "nubar";
- [χ] the uncertainties in the prompt fission neutron spectra.

Figure 4. Aggregate uncertainties for 4519 benchmarks calculated with NDaST for CIELO-1 and CIELO-2 actinide evaluations



Uncertainties are broken down into cross sections (σ), fission neutron yield (ν) and prompt fission neutron spectra (χ). The benchmarks are broken down by material and spectrum, with either a high-energy (FAST) spectrum or highly thermalised, lower-energy (THERM) spectrum. Average experimental uncertainties are shown in the background.

This meta-analysis, with each bar summarising averages over hundreds of simulations, shows that the application of the nuclear data covariances to any of a large number of different systems results in uncertainties with non-negligible differences. Several key differences between the aggregate CIELO-1 and CIELO-2 uncertainties were found in the calculation of uncertainties in integral k_{eff} criticality. These include:

- the use of IAEA standards for plutonium cross section uncertainties in CIELO-1 results in considerably larger uncertainties in plutonium k_{eff} than found with CIELO-2;

- the CIELO-2 HEU cross section uncertainties for fast systems are much larger than the IAEA standards used in CIELO-1;
- the PFNS uncertainties in highly enriched uranium (HEU) and plutonium systems for CIELO-2 are approximately twice those for the new CIELO-1 evaluations;
- nubar multiplicity (yield) uncertainties in CIELO-2 result in approximately 100 pcm higher uncertainties than with CIELO-1, for all systems except ^{233}U.

There are thus different subject matter experts making different (in some cases, very different) uncertainty assessments regarding knowledge of the fundamental data. A goal for future collaborative work is to understand, and possibly remove, these discrepancies.

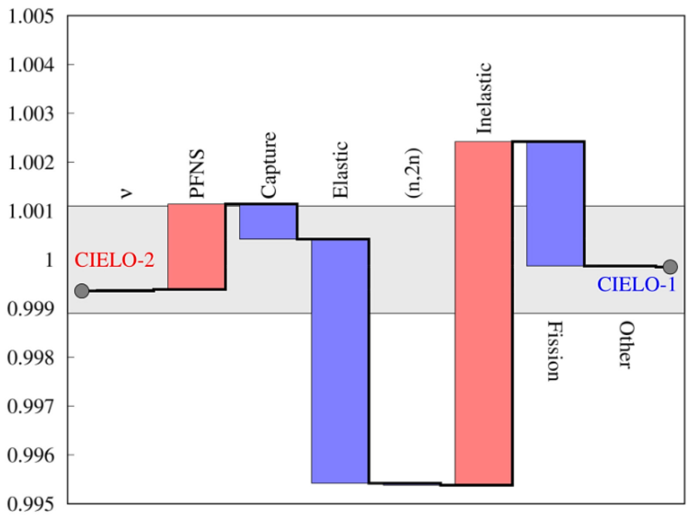
Discussion and conclusions

The Nuclear Energy Agency (NEA) Collaborative International Evaluated Library Organisation (CIELO) Pilot Project has been highly successful in bringing together experts from across multiple evaluation projects to collaborate in the production of new evaluated nuclear data files for several of the most influential isotopes. The new files that have been adopted by the ENDF/B-VIII.0 and JEFF-3.3 libraries improve performance in carefully selected criticality benchmarks, as well as in global testing. While considerable efforts were made to adopt evaluations with the standards of the International Atomic Energy Agency (IAEA), as well as harmonised with other data, it was recognised that independent evaluations from participating evaluation projects must be supported so as to allow choices to be made within the constraints established by experimental uncertainties.

While the evaluations are not identical, the results from the calculation of integral benchmarks show remarkable agreement between the results from both CIELO-1 and CIELO-2 evaluations. Figure 5 below shows the breakdown of the differences between the CIELO-1 and CIELO-2 evaluations for bare metal sphere benchmarks of ^{239}Pu (Jezebel) and ^{235}U (Godiva), respectively. In each case, switching one cross section between the two files has an effect that may be more than double the experimental uncertainty, yet the sum of all these is very close to zero. This trend is also highlighted in the uncertainty analyses shown in Tables 3 and 4 of this report. The combination of relatively large uncertainties and the need to find agreement on well-known benchmark simulations results in evaluations with differences that tend to compensate for each other. In the case of elastic and inelastic scattering, physical anti-correlations are the direct equivalent, and the apparent compensation in Figure 5 is simply a reflection of this well-motivated correlation. Some differences between evaluations may therefore only reflect selections within a distribution of equally justifiable evaluations, as constrained by experiment.

Uncertainties remain an area where harmonisation has not been as successful. It must be underlined that the evaluation of correlated uncertainties is a much more recent, and in many ways complex, addition to nuclear data files. Many parts of evaluated nuclear data files still do not possess any uncertainties, let alone full covariance matrices. The ongoing work within the NEA WPEC Subgroup 44 should contribute to progress on this topic, as well as other activities within the nuclear data evaluation projects.

Figure 5. Waterfall of the differences between the CIELO-2 (left) and CIELO-1 (right) evaluations in the simulation of the Jezebel bare plutonium sphere benchmark (PMF1)



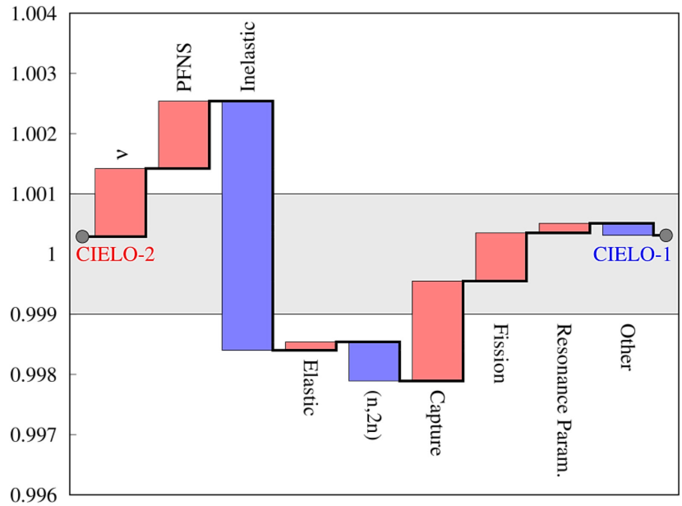
Contributions are broken down by components of the nuclear data file, including fission neutron yield (ν), prompt fission neutron spectra (PFNS) and various reaction cross sections. The experimental uncertainty is shown as a grey band. Each coloured band indicates the effect of substituting that component from the other evaluation.

Source: Adapted from *Nuclear Data Sheets* 148, February 2018: 189-213.

Several areas have been highlighted for further experimental data, including the continuation of some experimental campaigns carried out during the CIELO project, but on other high-priority isotopes. Notably, this includes the plutonium isotopes, including more work on ^{239}Pu, but while considering the other isotopes in parallel. Several other experiments are anticipated in the coming years and these would be well-paired with collaborative evaluation projects that will follow the success of the CIELO pilot.

Rapid processing and benchmarking were identified in this work as indispensable feedback. The availability of modern techniques and readily available computing power allows us to automate half of the evaluation-validation cycle. This was demonstrated with the NEA NDaST system, which automatically analysed thousands of datasets to provide prompt information to evaluators that historically took months to assemble. The expansion of its capabilities to include other neutronic parameters and sensitivities for even more systems will be essential for subsequent activities. The next phase of work will require us to take full advantage of this opportunity to integrate a processing and benchmarking framework for evaluators to receive immediate information on nuclear data files. The transformation of the file evaluation process (including all model codes, inputs and other expert guidance) into an automatable system remains the last challenge before we may fully close the evaluation-validation loop. With the rapid advancement of Big Data and Machine Learning techniques, the opportunity to apply them to a fully encapsulated nuclear data system would be one of the most natural directions to pursue.

Figure 6. Waterfall of the differences between the CIELO-2 (left) and CIELO-1 (right) evaluations in the simulation of the Godiva bare ^{235}U sphere benchmark (HMF1)



Contributions are broken down by components of the nuclear data file, including fission neutron yield (ν), prompt fission neutron spectra (PFNS), and various reaction cross sections. The experimental uncertainty is shown as a grey band. Each coloured band indicates the effect of substituting that component from the other evaluation.

Source: Adapted from *Nuclear Data Sheets* 148, February 2018: 189-213.

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Appendix A. About this publication

The Nuclear Energy Agency (NEA) would like to acknowledge the contribution of all of the scientists involved in the NEA Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 40 (SG40). In particular, the NEA wishes to express its gratitude to researchers and experts across different institutions who participated in WPEC SG40 meetings. The list of contributors can be found below. Oscar Cabellos and Michael Fleming provided valuable support in drafting and co-ordinating this report.

A CIELO collaboration team photo, from the kick-off meeting on 5-8 November 2013 in Geel, Belgium.

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International Co-operation in Nuclear Data Evaluation

Current knowledge of the nuclear physics of fuels and materials provides an understanding and simulation of the operations of nuclear reactors and other systems, both under ordinary and exceptional circumstances. As part of a broad spectrum of collaborative activities underpinning research in basic nuclear sciences, the Nuclear Energy Agency (NEA) is supporting collaboration between experimentalists, theoreticians and modelling experts to advance the state of the art in nuclear data.

This report offers an overview of collective results from 31 institutions in 15 NEA member countries, along with results from technical experts in the People's Republic of China, in the context of the NEA Collaborative International Evaluated Library Organisation (CIELO) Pilot Project. It reviews recent developments resulting from new measurements and semi-empirical models, as well as the validation of the CIELO nuclear data evaluations against suites of systems representing a wide range of current and future nuclear facilities. The CIELO project has delivered new, evaluated data for the isotopes of uranium, plutonium, iron, oxygen and hydrogen, which have been adopted in all nuclear data libraries released since the CIELO project was completed.

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